PB86-219086

Performance and Analysis of Aquifer Tests with Implications for Contaminant Transport Modeling

Auburn Univ., AL. Dept. of Civil Engineering

Prepared for

Robert S. Kerr Environmental Research Lab.
Ada, OK

Jul 86

U.S. Department of Commerce
National Technical Information Service
NTIS

PB86-219086

EPA/600/2-86/062
July 1986

PERFORMANCE AND ANALYSIS OF AQUIFER TESTS WITH IMPLICATIONS FOR CONTAMINANT TRANSPORT MODELING

by

Fred J. Molz, Oktay Güven, Joel G. Melville
Civil Engineering Department
Auburn University, AL 36849

and

Joseph F. Keely
Robert S. Kerr Environmental Research Laboratory
U.S. Environmental Protection Agency
P.O. Box 1198, Ada, OK 74820

CR-810704

Project Officer

Joseph F. Keely
Robert S. Kerr Environmental Research Laboratory
Ada, OK 74820

ROBERT S. KERR ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
ADA, OK 74820

REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U.S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA/600/2-86/062	2.
3. RECIPIENT'S ACCESSION NO. PB86 [illegible]/AS	
4. TITLE AND SUBTITLE PERFORMANCE AND ANALYSIS OF AQUIFER TRACER TESTS WITH IMPLICATIONS FOR CONTAMINANT TRANSPORT MODELING	5. REPORT DATE July 1986
	6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) F. J. Molz[a], Oktay Guven[a], Joel G. Melville[a], and Joseph F. Keely[b]	8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS [a]Civil Engineering Dept., Auburn Univ., AL 36849 [b]USEPA, R. S. Kerr Environmental Research Laboratory, P. O. Box 1198, Ada, OK 74820	10. PROGRAM ELEMENT NO. ABPC1A
	11. CONTRACT/GRANT NO. CR-810704
12. SPONSORING AGENCY NAME AND ADDRESS Robert S. Kerr Environmental Research Laboratory Office of Research and Development U. S. Environmental Protection Agency Ada, Oklahoma 74820	13. TYPE OF REPORT AND PERIOD COVERED Final
	14. SPONSORING AGENCY CODE EPA/600/15

15. SUPPLEMENTARY NOTES

Project Officer: Joseph F. Keely FTS: 743-2313

16. ABSTRACT

The scale-dependence of dispersivity values used in contaminant transport models to estimate the spreading of contaminant plumes by hydrodynamic dispersion processes was investigated and found to be an artifact of conventional modeling approaches (especially, vertically averaged parameters in two-dimensional plume simulations). The work reported here shows that variations in hydraulic conductivity with depth result in significant variations in ground-water flow and contaminant transport velocities; it is the resulting velocity variations that, if vertically averaged, give rise to apparant scale-dependency of dispersion (e.g., increased dispersion with increasing travel distance). Special depth-selective observation well designs are recommended by the authors for use in tracer tests, so that detailed estimates of the variations in hydraulic conductivity and flow and transport velocities can be obtained. Innovative modeling techniques, that take advantage of the detailed information obtainable from such tests (by emphasizing advective transport, as opposed to dispersive transport), have been developed by the authors. These modeling techniques are shown to have an element of true predictive ability, being able to closely simulate actual results with little or no calibration.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group

18. DISTRIBUTION STATEMENT	19. SECURITY CLASS *(This Report)*	21. NO. OF PAGES
RELEASE TO PUBLIC	UNCLASSIFIED	102
	20. SECURITY CLASS *(This page)*	22. PRICE
	UNCLASSIFIED	

EPA Form 2220-1 (Rev. 4-77) PREVIOUS EDITION IS OBSOLETE

DISCLAIMER

The information in this document has been funded wholly or in part by the United States Environmental Protection Agency under assistance agreement number CR-810704 to Auburn University. It has been subject to the Agency's peer and administrative review, and it has been approved for publication as an EPA document.

FOREWORD

The U.S. Environmental Protection Agency was established to coordinate administration of the major Federal programs designed to protect the quality of our environment.

An important part of the Agency's effort involves the search for information about environmental problems, management techniques and new technologies through which optimum use of the Nation's land and water resources can be assured and the threat pollution poses to the welfare of the American people can be minimized.

EPA's Office of Research and Development conducts this search through a nationwide network of research facilities.

As one of the facilities, the Robert S. Kerr Environmental Research Laboratory is the Agency's center of expertise for investigation of the soil and subsurface environment. Personnel at the laboratory are responsible for management of research programs to: (a) determine the fate, transport and transformation rates of pollutants in the soil, the unsaturated zone and the saturated zones of the subsurface environment; (b) define the processes to be used in characterizing the soil and subsurface environment as a receptor of pollutants; (c) develop techniques for predicting the effect of pollutants on ground water, soil and indigenous organisms; and (d) define and demonstrate the applicability and limitations of using natural processes, indigenous to the soil and subsurface environment, for the protection of this resource.

This report contributes to that knowledge which is essential in order for EPA to establish and enforce pollution control standards which are reasonable, cost effective and provide adequate environmental protection for the American public.

Clinton W. Hall

Clinton W. Hall
Director
Robert S. Kerr Environmental
Research Laboratory

Abstract

Due to worsening national problems, hydrologists are being asked to identify, assess or even anticipate situations involving groundwater contamination, and a large fraction of the regulation activities of the U.S. Environmental Protection Agency is in the groundwater area. In both regulation and assessment, increasing use is being made of complex mathematical models that are solved with the aid of a digital computer. Typically, such models are collections of partial differential equations that contain a number of parameters which represent aquifer physical properties and must be measured in the field. Of the various parameters involved, the hydraulic conductivity distribution is of major importance. Other parameters such as those relating to sorption, hydrodynamic dispersioon, and chemical/biological transformation are important also, but hydraulic conductivity is more fundamental because combined with head gradient and porosity it relates to where the water is moving and how fast. Therefore, this communication is devoted mainly to the conceptualization and measurement of hydraulic conductivity distributions and the relationship of such measurements to dispersion (spreading) of contaminants in aquifers.

For the most part, contemporary modeling technology is built around two-dimensional models having physical properties, such as transmissivity, that are averaged over the vertical thickness of the aquifer. In such a formulation, the major aquifer property related to contaminant spreading is forced to be longitudinal dispersivity. This is not due to any fundamental theoretical limitation. The major limitation is that dependable and economical field approaches for measuring vertically-variable hydraulic

conductivity distributions are not available. In the absence of such data, one has no choice in a modeling sense but to use some type of vertically-averaged advection-dispersion approach built around full aquifer longitudinal dispersivities.

In order to begin to overcome this limitation, a series of single-well and two-well tracer tests were performed at a field site near Mobile, Alabama, and a major objective of this communication is to describe these tracer tests and discuss some practical implications of the results with regard to modeling of contaminant dispersion in aquifers. The tests utilize multilevel sampling wells which have to be designed and installed carefully. Tracer test results along with theoretical studies suggest that the following working conclusions are warranted.

I. Local longitudinal hydrodynamic dispersion plays a relatively unimportant role in the transport of contaminants in aquifers. Differential advection (shear flow) in the horizontal direction is much more important.

II. The concept of full-aquifer dispersivity used in vertically-averaged (areal) models will not be applicable over distances of interest in most contamination problems. If one has no choice but to apply a full-aquifer dispersion concept, the resulting dispersivity will not represent a physical property of the aquifer. Instead, it will be an ill-defined quantity that will depend on the size and type of experiment used for its supposed measurement.

III. Because of conclusion II, it makes no sense to perform tracer tests aimed at measuring full-aquifer dispersivity. If an areal

model is used, the modeler will end up adjusting the dispersivity during the calibration process anyway, independent of the measured value.

IV. When tracer tests are performed, they should be aimed at determining the hydraulic conductivity distribution. Both our theoretical and experimental work have indicated that the variation of horizontal hydraulic conductivity with respect to vertical position is a key aquifer property related to spreading of contaminants.

V. Two- and three-dimensional modeling approaches should be utilized which emphasize variable advection rates in the horizontal direction and hydrodynamic dispersion in the transverse directions along with sorption and microbial/chemical degradation.

VI. In order to handle the more advection-dominated flow systems described in conclusion V, one will have to utilize or develop numerical algorithms that are more resistant to numerical dispersion than those utilized in the standard dispersion-dominated models.

Much of contemporary modeling technology related to contaminant transport may be viewed as an attempt to apply vertically homogeneous aquifer concepts to real aquifers. Real aquifers are not homogeneous, but they are not perfectly stratified either. What is being suggested, therefore, is that the time may have arrived to begin changing from a homogeneous to a vertically-stratified concept when dealing with contaminant transport, realizing fully that such an approach will be interim in nature and not

totally correct. Field calibration will still be required. However, the performance and simulation of several single- and two-well tracer tests suggests that the stratified approach is much more compatible with valid physical concepts, and at least in some cases results in a mathematical model that has a degree of true predictive ability.

An obvious implication of the study reported herein is that any type of groundwater contamination analysis and reclamation plan will be difficult, expensive and probably unable to meet all of the desired objectives in a reasonable time frame. Therefore, one can not overemphasize the advantages of preventing such pollution whenever it is feasible.

CONTENTS

Foreword iii
Abstract iv
Figures x
Tables xii

1. Introduction 1
   EPA's Site-Specific Modeling Efforts 2
   EPA's Generic Modeling Efforts 3
   Subsurface Transport Models 4
   The Hydraulic Conductivity Distribution 6
   The Mechanisms of Dispersion 9
   Simulation of Advection-Dispersion Processes 11
2. Types of Tracer Tests 18
3. Design and Construction of Multilevel Sampling Wells 23
4. Performance and Results of Single-Well and Two-Well Tracer Tests at the Mobile Site 37
   Single-Well Test 44
   Two-Well Test 52
5. Computer Simulation of Single-Well and Two-Well Test Results 61
   Simulation of Single-Well Tests 61
   Simulation of Two-Well Tests 68
6. Discussion and Conclusions 79

References 86

FIGURES

Number		Page
1	Hypothetical velocity distribution	14
2	Schematic diagram of contaminant concentrations	15
3	Vertical cross-sectional diagram of single well test	19
4	Two-well test geometry in a stratified aquifer	22
5	Various types of multilevel sampling systems	25
6	Pickens et al. multi-level sampling/observation well	26
7	Moltyaner and Killey multilevel, dry, access tube system for use with radioactive tracers	27
8	Schematic diagram of the basic construction plan for a multilevel sampling well with a removable insert	29
9	Multilevel sampling well with sampling zones isolated with inflatable packers and silicone rubber plugs	31
10	Details concerning the geometry and installation of inflatable packers	32
11	Diagram of a completed multilevel sampling well	33
12	Diagram illustrating the scheme for causing mixing in the various isolated sampling zones and obtaining samples for laboratory analysis	34
13	Diagram illustrating what may happen during drilling and installation of various types of screens	35
14	Possible beneficial effects of drilling mud left behind in the formation	36
15	Diagram of the subsurface hydrologic system at the Mobile site	39
16	Piping and valving scheme associated with pumping wells at the Mobile site	42
17	Diagram showing the main features of the surface hydraulic system used in the single- and two-well tracer tests at the Mobile site	43

18 Bromide concentration in the injection/withdrawal well (I2) 46

19 Bromide concentration breakthrough curves at the seven levels of well E3 during experiment #4 47

20 Electrical conductivity breakthrough curves at various levels of well E3 during experiment #4 48

21 Inferred normalized hydraulic conductivity distribution 53

22 Injection well tracer concentration versus time during the first 80 hours of the two-well test 56

23 Measured tracer concentration versus time in the withdrawal well during the two-well test 57

24 Measured and predicted breakthrough curves at the 7 levels of observation well E3 59

25 Normalized hydraulic conductivity distribution inferred from travel times measured during the two-well test 60

26 Hydraulic conductivity profile 63

27 Unsteady injection concentration during the Pickens and Grisak (1981) single-well field experiment . . . . . 6[illegible]

28 Comparison of SWADM results with field data for the flow-weighted concentration from an observation well one meter from the injection-withdrawal well 66

29 Comparison of SWADM results with field data for the flow-weighted concentration from an observation well two meters from the injection-withdrawal well 67

30 Comparison of SWADM results with field data for the concentration leaving the injection-withdrawal well 69

31 Results of various simulations of the two-well test 73

32 Calculated tracer concentration versus time in the withdrawal well 76

33 Comparison of measured and calculated tracer concentration versus time in the withdrawal well 78

34 Preliminary results of four single well tests performed at the Mobile site 83

TABLES

Number		Page
1	Particle size distribution data for the seven disturbed cores obtained during construction of well E3	41
2	Sampling zone elevations, arrival times for fifty percent breakthrough, apparent dispersivity values and inferred normalized hydraulic conductivity values for experiment #4	49
3	Two-well test parameters supplied to Geo-Trans, Inc. for their 3-dimensional simulations based on the advection-dispersion equation	71

Introduction

Due to worsening national problems and potential problems relating to industrial waste disposal, municipal waste disposal, radioactive waste disposal and others, there is increasing pressure on hydrologists to identify, assess or even anticipate situations involving groundwater contamination. In order to meet these demands, subsurface hydrologists have turned increasingly to the use of complex mathematical models that are solved with the aid of a digital computer. Some of the principal areas where mathematical models can now be used to assist in the management of EPA's groundwater protection programs are:

(1) appraising the physical extent, and chemical and biological quality, of groundwater reservoirs (e.g., for planning purposes),

(2) assessing the potential impact of domestic, agricultural, and industrial practices (e.g., for permit issuance, EIS's, etc.),

(3) evaluating the probable outcome of remedial actions at hazardous waste sites, and of aquifer restoration techniques generally,

(4) providing exposure estimates and risk assessments for health-effects studies, and

(5) policy formulation (e.g., banning decisions, performance standards).

These activities can be broadly categorized as being either site-specific or generic modeling efforts, and both categories can be further subdivided into point-source or nonpoint-source problems. The success of these efforts depends on the accuracy and efficiency with which the natural processes controlling the behavior of groundwater, and the chemical and biological species it transports, are simulated. The accuracy and efficiency of the simulations, in turn, are heavily dependent on the applicability of the

assumptions and simplifications adopted in the model(s), and on subjective judgments made by the modeler and management.

EPA's Site-Specific Modeling Efforts

Whether for permit issuance, investigation of potential problems, or remediation of proven contamination, site-specific models are necessary for the Agency to fulfill its mandate under a number of major environmental statutes. The National Environmental Policy Act (1970) stipulates a need to show the impact of major construction activities in Environmental Impact Statements and potential impacts are often projected by the use of mathematical models. The Underground Injection Control (UIC) program, which originated in the Safe Drinking Water Act (1974) (SDWA) and is now subject to provisions of the Resource Conservation and Recovery Act (1984 Amendments) (RCRA), requires an evaluation of the potential for excessive pressure build-up and contaminant movement out of the injection zone. Mathematical models are the primary mechanism for the required evaluation, due in part to the difficulty of installing monitoring wells several thousand feet deep.

UIC also calls for determinations of which aquifers serve, or could serve, as underground sources of drinking water (USDW's), based on a lower quality limit of 10,000 ppm total dissolved solids. Here, modeling has been found to be a useful adjunct to gathering and interpreting field data, such as in the U.S. Geological Survey's efforts to assist EPA in determining USDW's (e.g., the RASA program). Another SDWA program, for the designation of Sole Source Aquifers (SSA), has frequently employed the use of models for establishing and managing water-quality goals. Designation of the Spokane

Valley - Rathdrum Prairie SSA, for instance, included an evaluation of nonpoint-sources of nitrates with a groundwater model developed for EPA by the USGS.

Some of the most difficult site-specific problems facing the Agency involve hazardous waste sites falling under the purviews of RCRA and CERCLA/Superfund. Associated with most of these sites is a complex array of chemical wastes and the potential for groundwater contamination. Their hydrogeologic settings usually appear quite complicated when examined at the scale appropriate for technical assessments and remediation efforts (e.g., 100's to 1000's of feet). Groundwater models are used to assist in the organization and interpretation of data gathered during remedial investigations, the prediction of potential contaminant transport pathways and rates of migration, the setting of Alternate Concentration Limits, the design and comparison of remedial alternatives, and the evaluation of the performance of final ('as built') designs at hazardous waste sites. They are also used to help determine the adequacy of monitoring and compliance networks, and to determine the feasibility of meeting clean-up targets.

EPA's Generic Modeling Efforts

There are a number of instances where the Agency has limited data or other constraints, such that site-specific modeling is not feasible. As a result, many decisions are made with the assistance of generic modeling efforts. Generic efforts utilize analytical models, as opposed to numerical models, to a much greater degree than occurs in site-specific efforts. This is a logical consequence of the simplified mathematics of analytical models,

the significantly greater data requirements of numerical models, and the higher costs of numerical simulations.

The Agency has many statutory responsibilities which benefit from generic modeling, including the estimation of potential environmental exposures, and their integration with dose-response models to yield health-based risk assessments. These are necessary, for example, in issuing compound-specific rulings on products subject to pre-registration requirements under the Toxic Substances Control Act and the Federal Insecticide, Fungicide, and Rodenticide Act. More generalized policy formulation activities also benefit from generic modeling efforts. Examples include making policy decisions about land disposal 'banning,' preparing Technical Enforcement Guidance Documents (i.e., for monitoring network designs), and 'delisting' under RCRA.

Subsurface Transport Models

The most common types of modern groundwater transport models are a collection of partial differential equations and other mathematical/physical relationships that embody our best understanding of the system of interest, which in the present context is an aquifer. Virtually all groundwater models contain a number of parameters, which are simply numbers or functions that represent the physical and chemical properties of an aquifer and the aqueous solution that it contains. In order to apply a model to a particular problem situation, one must specify all the parameters (length, width, thickness, hydraulic conductivity, dispersivity, retardation coefficient, etc.) that pertain to that particular system. This is what

distinguishes one system from another in the application of a mathematical model.

In the actual process of using a mathematical model, the user puts all necessary information into the model (geometry, physical properties, initial and boundary conditions), and a computer is employed to rapidly solve the resulting equations which generates the model output. Output, for example, might include a predicted contaminant concentration distribution 10 years in the future. Presently, this predictive process is far from satisfactory (Konikow, 1986). Our understanding of all the physical and chemical phenomena involved is imperfect, and there are immense difficulties in measuring and specifying all of the required input data. If accurate information is not put into a mathematical model, one cannot expect accurate information to come out.

Over the past decade, a significant number of scientists have concluded that the single most important barrier to developing an improved ability to simulate groundwater contamination problems is our inability to measure, specify and, therefore, understand the type of hydraulic conductivity distribution that occurs in natural aquifers (Smith and Schwartz, 1981). This is not to say that other parameters such as those relating to sorption, hydrodynamic dispersion and chemical/biological transformations are not important. It is simply that the hydraulic conductivity is more fundamental, because together with the hydraulic head distribution and porosity, it is the physical property that relates to where and how fast the groundwater is moving. If one does not have the ability to specify the location of a parcel of water at a given time, one can hardly specify what

is going on chemically and biologically in that water. Therefore, this communication is devoted mainly to the conceptualization and measurement of hydraulic conductivity distributions and the relationship of such measurements to dispersion (spreading) of contaminants in aquifers.

The Hydraulic Conductivity Distribution

Measurement of hydraulic conductivity is difficult because of aquifer location (i.e., below the ground surface) and the nonhomogeneity of most natural aquifers. (It is not uncommon for hydraulic conductivity to vary by a factor of 10^8 or more within a given subsurface hydrologic system (Freeze and Cherry, 1979).) As discussed by Schwartz (1977), almost a continuously increasing scale of heterogeneity can be visualized in most aquifers. The heterogeneities arise due to variations in grain sizes and pore sizes, permeability trends due to stratification and variations in the original depositional environment, anisotropy, fractures, overall stratigraphic framework and more (Alpay, 1972). Because of the range of many of these variations and the unique physical, chemical and biological environments found in the subsurface, it is difficult or impossible to study spatial variability in a definitive way with laboratory experiments.

According to Philip (1980) field heterogeneity can be classified as either deterministic or stochastic. Deterministic heterogeneity refers to hydraulic conductivity variations that are sufficiently ordered to be characterized by a set number of measurements, although in practice the measurements may be difficult to make. Stochastic heterogeneity refers to hydraulic conductivity changes that are essentially random, making it pointless to try to measure them all. However, even these categories depend

on scale of observation (problem size), because variations that can be viewed collectively as stochastic on a sufficiently large scale (regional scale) may have to be treated as deterministic on a smaller scale such as a site-specific scale. In addition, stochastic variations are often embedded in systematic trends (i.e., random variations within discrete strata).

Since a complete characterization of the spatial distribution of hydraulic conductivity and hence a complete description of all the details of the flow field in an aquifer are practically impossible, various stochastic convection-dispersion models for solute transport have been proposed in recent years (e.g., Gelhar and Axness, 1983; Winter, 1982). While these models may be useful under certain conditions, they also have various limitations. Detailed discussions of the capabilities and limitations of these models may be found in Gelhar et al. (1979), Matheron and deMarsily (1980), Gelhar and Axness (1983), Dagan (1984), and Sposito, Jury and Gupta (1986). As reviewed in detail in the recent paper by Sposito, Jury and Gupta (1986), all such models involve a conceptual collection (ensemble) of statistically similar aquifers rather than a specific real aquifer. Consequently, these stochastic models provide results which are averages over the collection and, therefore, not directly applicable to a single aquifer. In addition, only under very limited conditions can measurements in a single real aquifer be related even conceptually to the statistics of a collection of aquifers that contains the real aquifer as one of its members. Essentially, the real aquifer must be statistically homogeneous on the average and ergodic (Neuman, 1982; Sposito, Jury and Gupta, 1986). Without going into details here, it is sufficient to

say that such a condition is very restrictive and does not allow an aquifer to have the type of general variability and persistent hydraulic conductivity trends that we believe are essential to understanding contaminant transport, particularly in site-specific situations involving relatively short travel distances. For these reasons and others, Sposito, Jury and Gupta (1986) concluded that "much more theoretical research is required and the stochastic convection-dispersion model does not yet warrant unqualified use as a tool for physically based, quantitative applications of solute transport theory to the management of solute movement at field scales."

In order to circumvent the fundamental difficulties of the stochastic convection-dispersion approach discussed in the previous paragraph and to deal at the same time with the problem of prediction uncertainty caused by data limitations, Smith and Schwartz (1981) (see also Dagan, 1984) have suggested the use of conditional simulations, a technique originally developed in the field of geostatistics (see, e.g., Journel and Huijbregts, 1978). Recent developments in the application of geostatistical estimation methodology in the groundwater field (Kitanidis and Vomvoris, 1983; Hoeksema and Kitanidis, 1984) make this approach promising. The geostatistical conditional simulations approach allows one to make direct use of all the available field data in solute transport predictions for a given aquifer, and also to provide estimates of the uncertainty in these predictions. Using this technique, the known features of the aquifer and the flow are taken into account in a deterministic manner while the unknown features are approximated and dealt with in a probabilistic manner. A major difference between this approach and the stochastic convection-dispersion model is that

the geostatistical methodology takes into account the actual spatial variations of aquifer properties by conditioning the simulations on the available measurements while the aforementioned stochastic models make use of the available data only to estimate the statistical structure of the assumed aquifer collection (ensemble). In fact, the results provided by the stochastic models referred may be viewed as being equivalent to the averages of the results which would be provided by unconditional simulations of the geostatistical approach. Due to the lack of conditioning, considerable uncertainty may exist in the predictions of the stochastic models when compared with the predictions of conditional simulations as indicated by the results of Smith and Schwartz (1981) and Güven (1986). While the geostatistical approach does appear promising in dealing with problems of solute transport, it is presently at an early stage of development and considerable theoretical work, improved numerical procedures, improved field measurement techniques and field verification studies are needed before any routine application of this approach in the field would be practical. In the meantime, interim approaches are required to advance our capability of modeling solute transport. More will be said about one such interim approach later.

The Mechanisms of Dispersion

In order to improve our capability of modeling solute transport, it is very important to understand the major physical mechanisms which affect the evolution and probable future of an existing groundwater contamination plume or the future course of an anticipated plume. The catch-all name given to the spreading of a contaminant in groundwater is dispersion, a term which is

familiar to almost everyone. However, as illustrated in Figure 1, many different phenomena contribute to the dispersion process in aquifers. The horizontal extent of the hypothetical tracer plume in Figure 1 is determined mainly by the elapsed travel time and the difference between the maximum and minimum values of the horizontal advective velocities. These velocity variations result primarily from the variations of hydraulic conductivity. Dilution within the plume and along the plume boundaries is caused by pore-scale mixing (local hydrodynamic dispersion) due in part to molecular diffusion, velocity variations within each pore, and the overall tortuosity of the flow path. In the hypothetical situation depicted in Figure 1, there is an overall trend of hydraulic conductivity increase from the top towards the bottom of the aquifer. Four minor trends, resulting in hydraulic conductivity peaks in both the upper third and bottom third of the aquifer, are evident also, with the lower peak being more pronounced. The plume concentration distribution is determined to a large extent by these trends. In addition, there are "wobbles" in the concentration distribution caused by seepage velocity components in all directions at a scale smaller than the scale of the minor trends noted above. Thus the actual concentration distribution of the plume is determined by a combination of strata-scale advective effects arising from the nonuniform velocity distribution and pore-scale mixing effects caused by the concentration differences within the plume and the basic nature of pore-scale flow. This pore-scale effect is most pronounced at the plume boundaries because the concentration gradients are largest there. In addition, wobbles in the concentration distribution at an intra-stratum scale could, after a sufficient travel time, result in a type of semi-local mixing, which some researchers have called macro-dispersion (Gelhar and Axness, 1983). As the plume travels further

downstream, the concentration gradients in the transverse direction would be gradually smoothed out due to both hydrodynamic dispersion and seepage velocity components in the transverse direction and a somewhat well-mixed condition would develop at each streamwise station over the whole depth of the aquifer after a sufficiently long travel time. However, the time required for this behavior could be very large (see, e.g., Gelhar et al., 1979; Matheron and deMarsily, 1980; Molz et al. 1983; Güven et al., 1984). In many site-specific situations, such large travel times are usually not involved, and variations of concentration over the depth of the aquifer are expected to be an important consideration when dealing with particular site-specific problems.

Simulation of Advection-Dispersion Processes

Historically, the field of subsurface hydrology developed mainly in response to groundwater supply problems. To solve such problems there was often little need to develop detailed information concerning the spatial variability of hydraulic conductivity within a given aquifer. Knowledge of the average transmissivity and storativity of the aquifer was adequate along with specification of the vertical aquifer boundaries (water table or confining layers) and in some cases the lateral boundaries. For these conditions, one-dimensional, horizontal, transient flow in a confined homogeneous aquifer may be written as (Freeze and Cherry, 1979)

$$\frac{\partial^2 h}{\partial x^2} = \frac{S}{T}\frac{\partial h}{\partial t} \qquad (1)$$

where x = length in the direction of flow, t = time, h = hydraulic head, S = storativity and T = transmissivity. Typically, the average S and T values would be determined by a pumping test utilizing fully-screened, fully-penetrating pumping and observation wells (Freeze and Cherry, 1979).

More recently, when societal trends shifted from groundwater supply to groundwater contamination problems, it seemed logical to work with the contaminant transport version of equation (1). For steady horizontal flow but transient (time changing) dispersion of a conservative solute in a confined aquifer, this equation is given by (Freeze and Cherry, 1979)

$$\frac{\partial c}{\partial t} + V \frac{\partial c}{\partial x} = D_L \frac{\partial^2 c}{\partial x^2} \qquad (2)$$

where c = solute concentration, V = uniform seepage velocity and D_L = longitudinal dispersion coefficient. D_L is given by the product $\alpha_L V$, where α_L is the longitudinal dispersivity, which represents the random local mixing properties of the aquifer. But what happens if one attempts to blindly apply equation (2) to the situation depicted in Figure 1? First of all, one would have to work with some average horizontal velocity, $\bar{V}$, an average concentration, $\bar{c}$, and some type of apparent or effective dispersion coefficient, D_L^*, which we will call the "full aquifer" dispersion coefficient. With these assumptions, solutions of equation (2) would predict tracer distributions similar to those shown in Figure 2. Comparison of the predicted distributions (which, as a result of the assumptions are uniform in the vertical direction) with the more realistic distribution (Figure 1B) shows this approach to be generally unsatisfactory. A lot of useful information has been lost by not incorporating the vertical distribution of hydraulic conductivity. This example highlights the problem that results when attempting to solve groundwater contamination problems with approaches found to be useful in water supply problems. Two-dimensional versions of equation (2) are the so-called areal advection-dispersion models; they are based on the same vertically-averaged approach and thus suffer from the same limitations.

If one considers explicitly the vertical variation of hydraulic conductivity for the transport problem illustrated in Figure 1 with flow, V(z), parallel to the stratification in a horizontal stratified aquifer, the governing equation becomes (Molz, Güven and Melville, 1983)

$$\frac{\partial c}{\partial t} + V(z)\frac{\partial c}{\partial x} = D_L(z)\frac{\partial^2 c}{\partial x^2} + \frac{\partial}{\partial z}(D_T(z)\frac{\partial c}{\partial z}) \qquad (3)$$

where $c = c(x,z,t)$ = concentration distribution, z = vertical coordinate, $D_T = \alpha_T V(z)$ = transverse (vertical) dispersion coefficient, $D_L = \alpha_L V(z)$ = longitudinal dispersion coefficient, α_T = local transverse (vertical) dispersivity and α_L = local longitudinal dispersivity. If D_L is small, as is often the case (Pickens and Grisak, 1981), one can neglect, without much error, the local longitudinal mixing term in equation (3) which leaves (Güven et al., 1984)

$$\frac{\partial c}{\partial t} + V(z)\frac{\partial c}{\partial x} = \frac{\partial}{\partial z}(D_T(z)\frac{\partial c}{\partial z}) \qquad (4)$$

While the local longitudinal mixing term may be neglected, the local transverse mixing term has a very important influence on the solute spreading, particularly at intermediate and large times (Molz et al., 1983; Güven et al, 1984). Noting that by identity $V(z) = \bar{V} + (V(z) - \bar{V})$, one can write equation (4) as

$$\frac{\partial c}{\partial t} + \bar{V}\frac{\partial c}{\partial x} = \frac{\partial}{\partial z}(D_T(z)\frac{\partial c}{\partial z}) - (V(z)-\bar{V})\frac{\partial c}{\partial x} = \frac{\partial}{\partial z}(D_T(z)\frac{\partial c}{\partial z}) - \frac{\partial}{\partial x}((V(z)-\bar{V})c) \qquad (5)$$

In this form it is particularly illuminating to compare equations (2) and (5), because one can see in mathematical/physical terms an implication of the discrepancy illustrated graphically in Figures 1 and 2. If one forces equation (2) to fit a dispersion process properly described by equation (5), then the full aquifer dispersion term will have to model solute spreading

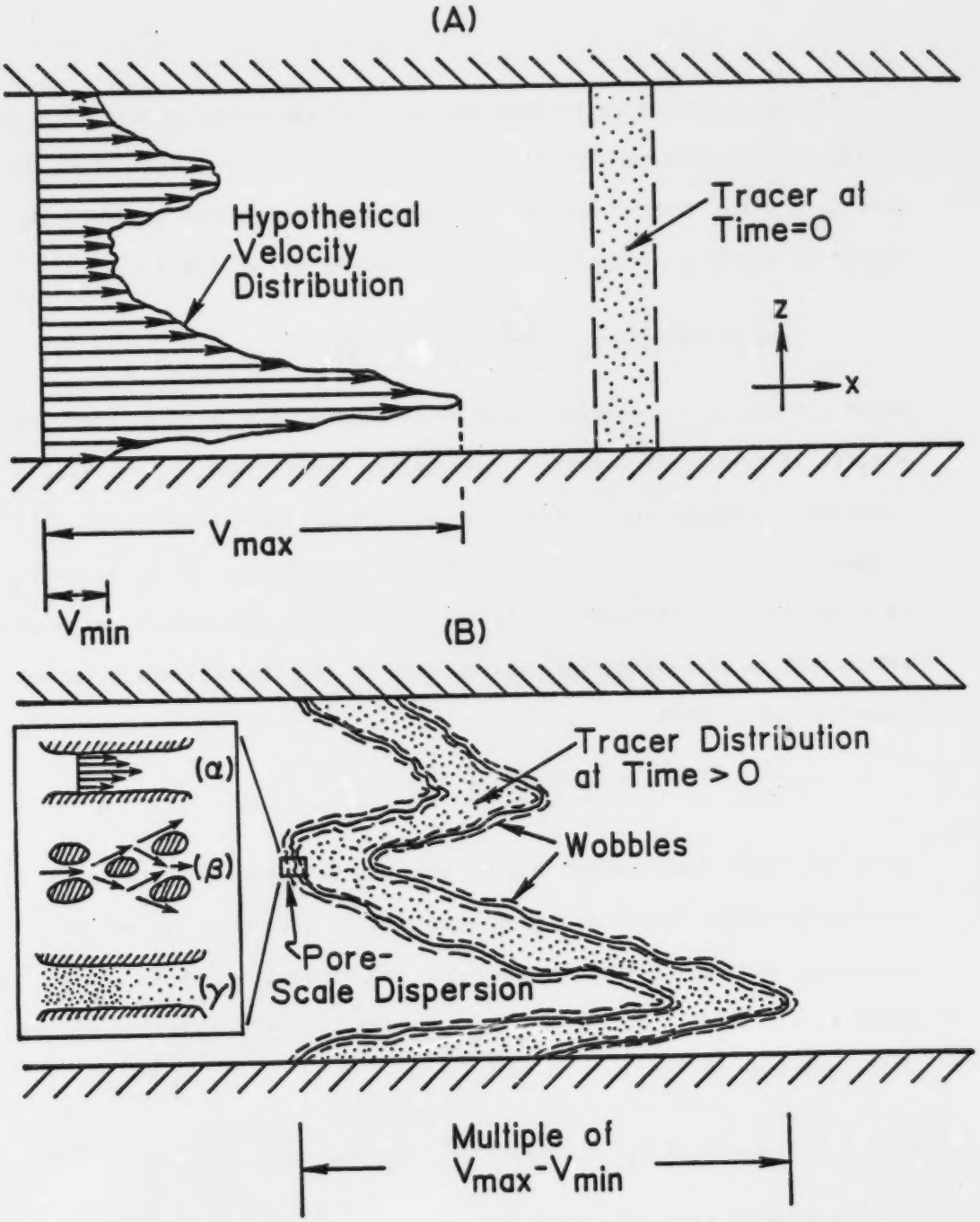

Figure 1. Part (A) shows a hypothetical velocity distribution and an initial distribution of tracer while part (B) shows how the tracer would be dispersed by the moving groundwater at several different scales. Three common mechanisms of pore scale dispersion (velocity variation within a pore (α); flow path tortuosity (β), and molecular diffusion due to concentration differences (γ)) are illustrated also.

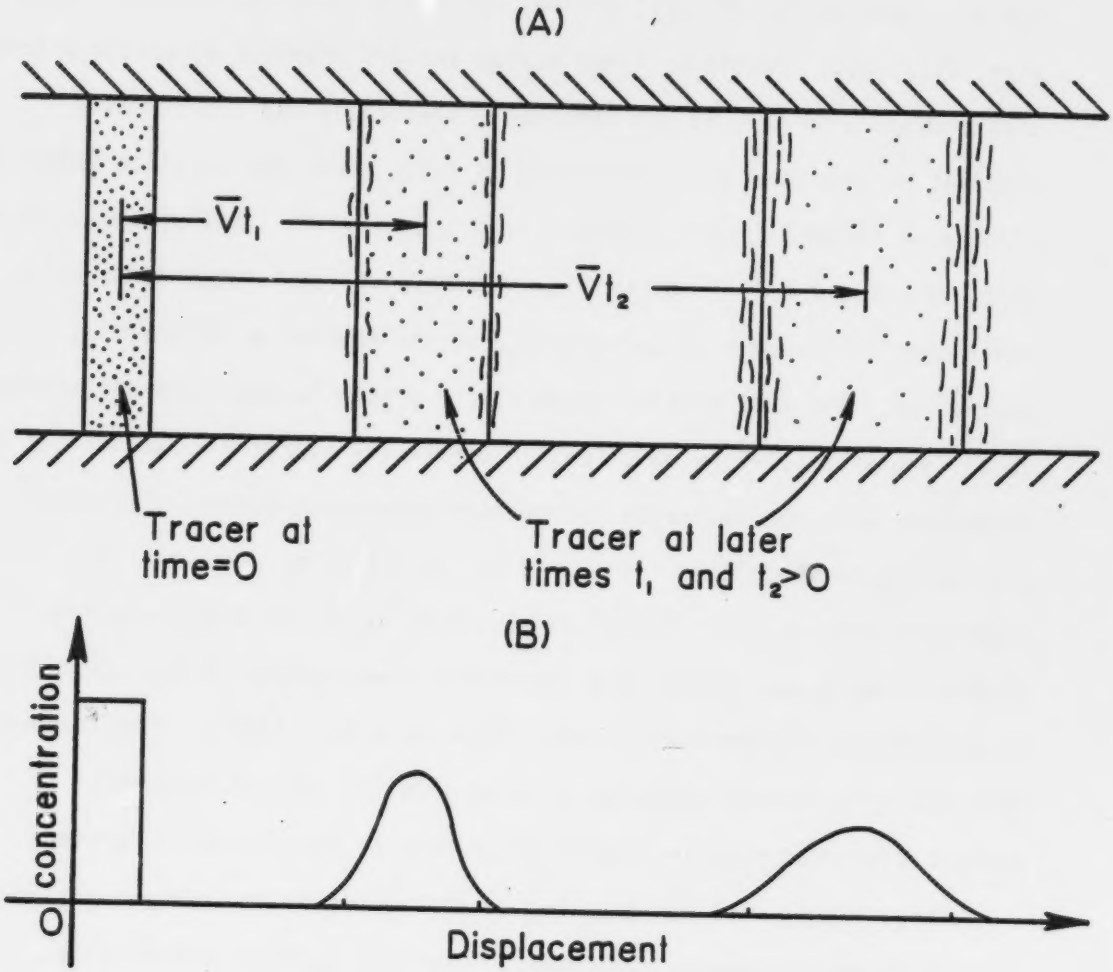

Figure 2. Schematic diagram showing the inherent lack of vertical contaminant concentration structure resulting from vertically-averaged transport models (part A) and the resulting plots of concentration versus distance (part B).

due to a combination of local mixing, $D_T(z)\partial c/\partial z$, and differential advection, $(V(z)-\bar{V})c$. Combining local mixing and differential advection within a single dispersion term is not reasonable physically and not strictly possible mathematically, as discussed by Molz, Güven and Melville (1983) and elaborated in more detail by Güven, Molz and Melville (1984). The overall approach makes the full-aquifer dispersivity, α_L^*, scale-dependent, which means that it is not a unique property of the aquifer or of anything else in particular. The full-aquifer dispersivity simply becomes a parameter used to fit equation (2)-type solutions to vertically-averaged concentration distributions when the desirable information concerning hydraulic conductivity profiles is not available. Not only is the fit often poor, but the numerical size of such "fitted" dispersivity values is usually several orders of magnitude larger than laboratory measurements of true hydrodynamic dispersivities (Pickens and Grisak, 1981; Anderson, 1983). This suggests that the differential advection arising from the overall hydraulic conductivity distribution plays a major role in the dispersion process.

These remarks are not provided simply to discredit areal advection-dispersion models because such models have been applied productively. However, the fitting process associated with the identification of full-aquifer dispersivity values means that the use of such models as truly predictive tools is highly questionable. Their success to date has been severely limited by the non-unique and ill-defined nature of the full-aquifer dispersivity. Partly because of this, examination of down-gradient impacts of a contaminant plume usually requires major re-calibration of a full-aquifer model developed for the local site. Despite these limitations, areal advection-dispersion models continue to serve a useful purpose because of the lack of adequate and practical field

techniques for determining the hydraulic conductivity distribution. Only recently have experiments with the objective of measuring vertical distributions of horizontal hydraulic conductivity been performed (Pickens and Grisak, 1981; Molz et al., 1985, 1986). Thus the required instrumentation and testing techniques are neither fully developed nor widely available. In the absence of vertically-distributed data, one has no choice in a modeling sense but to use some type of vertically-averaged advection-dispersion approach built around full aquifer dispersivities. However, we believe that much more can be done with existing instrumentation and techniques than is typically done during field investigations of groundwater contamination incidents.

As supported by the previous arguments, it is likely that any real advance in our ability to simulate the contaminant dispersion process in aquifers will have to be built upon more detailed measurements of hydraulic conductivity and head distributions so that the advection field is defined in more detail. It is particularly important to move away from the exclusive use of vertically-averaged aquifer properties and flow variables. Recently, we have performed single-well and two-well tracer tests at a site near Mobile, Alabama with the objective of measuring relative travel time distributions across the vertical dimension of an aquifer, assuming horizontal flow on the average. We conducted those experiments because tracer tests provide the most definitive data with which to infer hydraulic conductivity distributions. A major purpose of this communication is to describe these tracer tests and testing procedures and to discuss some practical implications of the results with regard to modeling of contaminant dispersion in aquifers.

Types of Tracer Tests

It is generally agreed that tracer tests are currently the most reliable field methods for obtaining data to describe dispersion in groundwater. Most tracer tests can be placed in two major categories--natural gradient and forced gradient. As the name implies, natural gradient tests involve various means of placing an inert, non-adsorbing chemical (tracer) in an aquifer and allowing it to move with the natural groundwater flow (Sudicky, Cherry and Frind, 1983). Stanford University, in cooperation with the University of Waterloo, has recently completed a detailed natural gradient test soon to be reported in Water Resources Research. Herein we are concerned mainly with forced gradient tests which employ pumping wells (injection and/or withdrawal) to move a tracer through the test aquifer. Normally, the selected pumping rates are such that the resulting hydraulic gradients are much larger than the natural gradient. For this reason, forced gradient tests are much shorter in duration than natural gradient tests. The most common types of forced gradient tracer tests are single-well tests and two-well tests. Over the past two years, both types have been performed at the Mobile site (Molz et al., 1985, 1986), and both types have been studied in some theoretical detail relative to their analysis and interpretation in stratified aquifers (Güven et al., 1985, 1986). The stratified aquifer assumption represents the simplest aquifer idealization having a horizontal hydraulic conductivity distribution that depends on the vertical coordinate (Güven, Molz and Melville, 1984).

Shown in Figure 3 is a typical configuration for a single-well test. The term "single-well" represents the fact that only one pumping well is required in order to perform the test. As detailed in Güven et al. (1985), an observation well with multilevel samplers is required in order to obtain

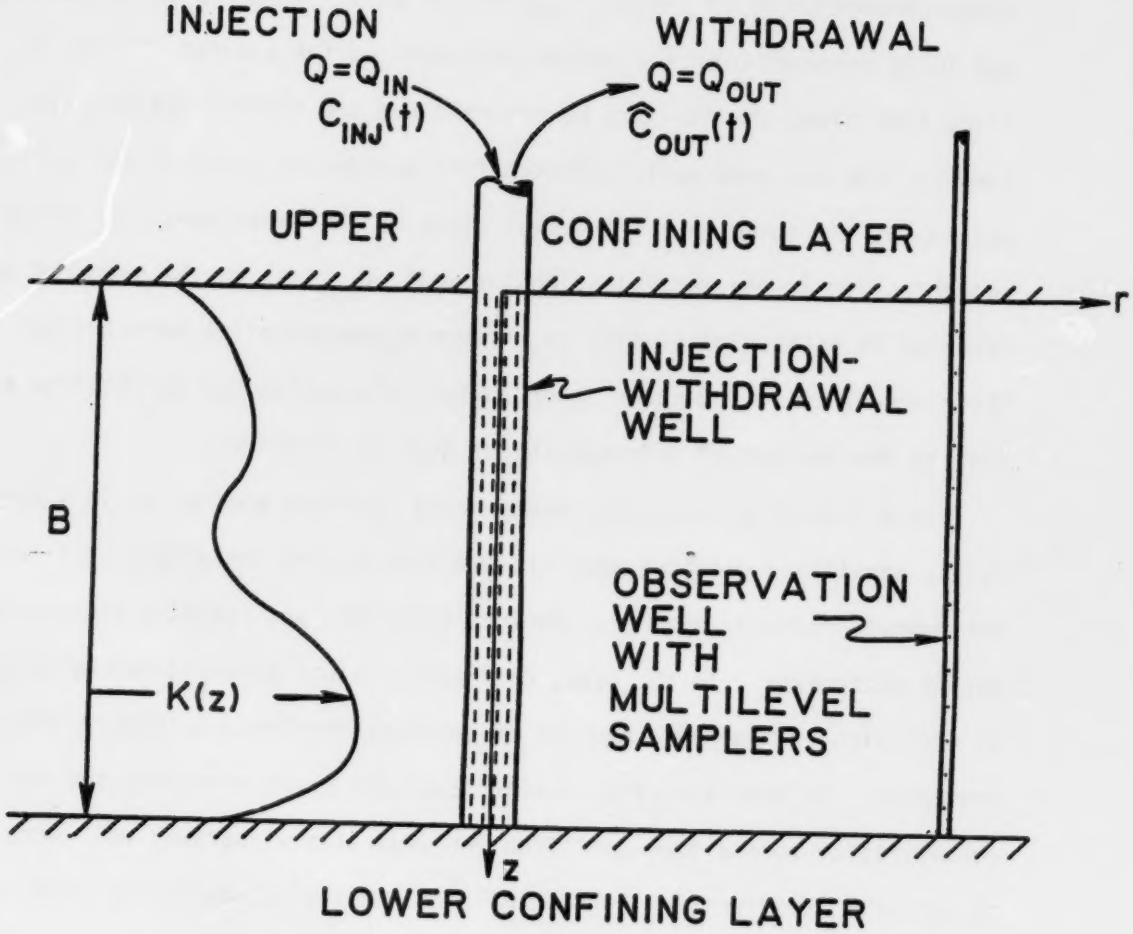

Figure 3. Vertical cross-sectional diagram showing single-well test geometry.

tracer travel time data at several vertical positions in the aquifer. One or more such observation/sampling wells may be used in any particular tracer test. Actual test performance involves the injection of water having a known concentration of tracer, $C_{inj}(t)$, in a well which is fully penetrating and fully screened over the entire thickness of the aquifer (Figure 3). After some time, the flow may be reversed and the tracer-labeled water removed from the same well, although this withdrawal phase is not strictly necessary. If there is a withdrawal phase in the experiment, the tracer concentration in the water leaving the well, $\hat{C}_{out}(t)$, may be measured and recorded as a function of time to produce a concentration versus time breakthrough curve. Certain other useful information may be obtained also such as the percent of injected tracer that is recovered.

In a laterally isotropic, homogeneous confined aquifer or in a perfectly stratified confined aquifer, the flow during the single-well test is horizontal, radially diverging during injection, and radially converging during withdrawal. In the past, data analysis was accomplished by assuming an equivalent homogeneous aquifer of constant thickness B (Fig. 3 with K(z) constant). In such analyses, a withdrawal phase was necessary and the concentration versus time data from the injection-withdrawal well were used to estimate an effective longitudinal full-aquifer dispersivity (see, e.g., Fried, 1975; Pickens and Grisak, 1981). As mentioned previously, we believe that an approach which does not rely on the vertically homogeneous aquifer assumption is more reliable for predictive purposes.

In the single-well tests to be discussed, one or more observation wells containing isolated multilevel sampling devices are installed around the injection-withdrawal well (Fig. 3). Concentration versus time measurements are then made at the different isolated points in each observation well

during the experiment. The resulting tracer travel time information may be used to infer vertical profiles of horizontal hydraulic conductivity. When a single-well test is performed in this manner, the data from the multilevel observation well(s) is what one is after. Therefore, a withdrawal phase is not strictly necessary but is recommended, if for no other reason than to remove tracer from the study aquifer.

A typical configuration and flow pattern for a two-well tracer test is illustrated in Figure 4. Here there are two pumping wells because the experiment involves the simultaneous operation of an injection well and a withdrawal well, both of which are fully screened and fully penetrating over the entire thickness of the aquifer. Water is pumped into the injection well at a steady flow rate, Q, and is removed from the withdrawal well, usually at the same rate, although two-well tests have been performed in which the flow rates in the two pumping wells were not equal (e.g., Gelhar, 1982). A conservative tracer of known concentration, $C_{in}(t)$, is added at the injection well for a period of time, t_{in}, and the concentration of tracer in the water leaving the withdrawal well, $\hat{C}_{out}(t)$, is measured and recorded as a function of time to give a concentration versus time breakthrough curve. The tracer injection period is usually short compared to the total time of the experiment.

Two-well tests may be carried out in either a recirculating or non-recirculating mode. In the recirculating mode, the water pumped from the withdrawal well is piped to the injection well, where it is injected back into the aquifer. The concentration of tracer entering the injection well during a two-well test with recirculation, $C_{inj}(t)$, will be equal to $C_{inj}(t) = C_{in}(t) + \hat{C}_{out}(t)$, approximately, assuming that the travel time in the pipe joining the two wells is negligible. In the non-recirculating

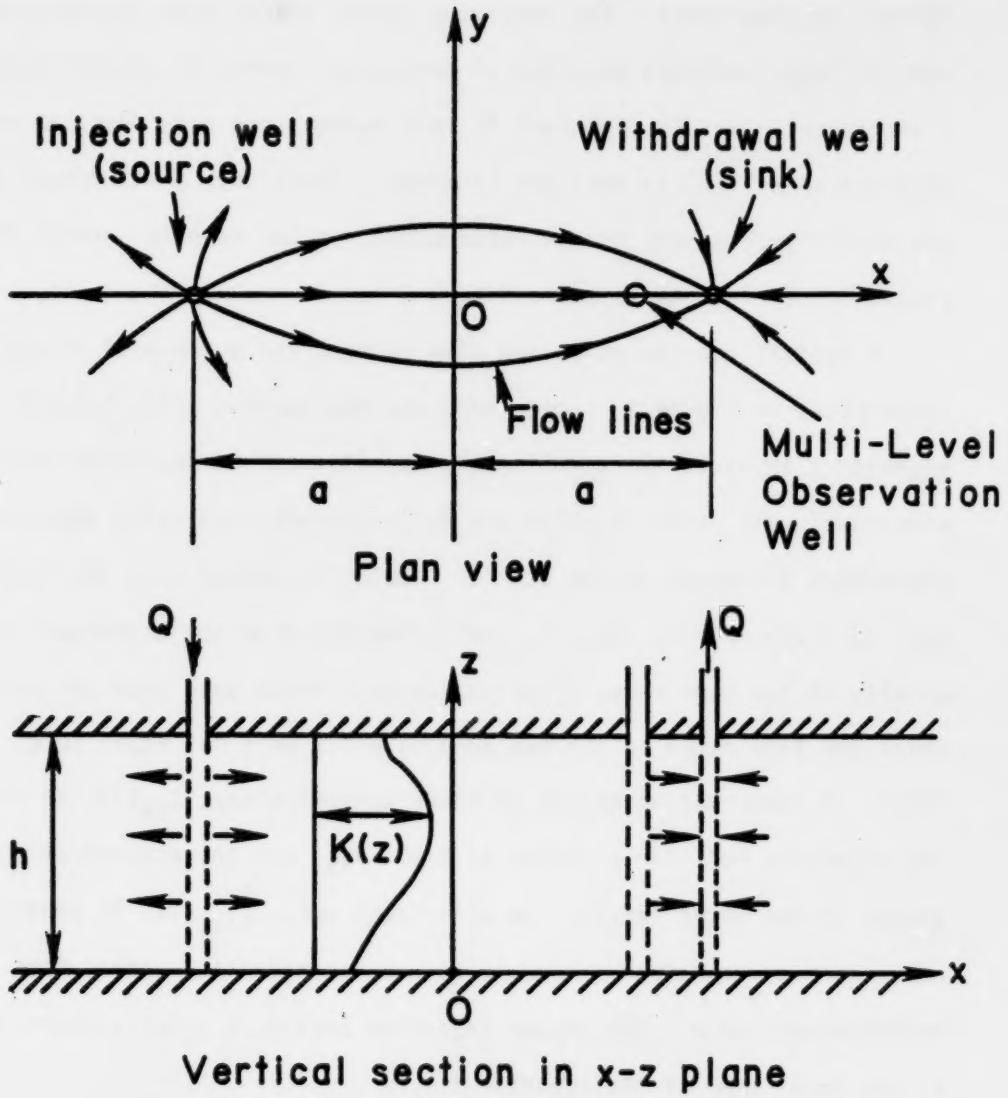

Figure 4. Two-well test geometry in a stratified aquifer.

mode, the water produced from the withdrawal well is wasted at a safe distance from the test area. A separate water supply, usually a well in the same aquifer but sufficiently far from the two test wells, so that negligible hydraulic interference occurs, provides the injection water. The injection tracer concentration in this case is $C_{inj}(t) = C_{in}(t)$.

For the two-well tests discussed herein, observation wells containing isolated multilevel samplers are installed between the injection well and the withdrawal well in order to sample the tracer concentration at different elevations in the aquifer during the experiment. From the tracer arrival times at several isolated sampling points in a multilevel sampling observation well, the variation of horizontal hydraulic conductivity in the vertical may be inferred (Pickens and Grisak, 1981). As will be described in more detail later, the inference assumes that the aquifer is perfectly stratified and of constant thickness and porosity in the vicinity of the test wells.

Design and Construction of Multilevel Sampling Wells

As explained in the previous section, the most unique aspect of the single- and two-well tests that we are discussing is the use of one or more multilevel sampling wells to obtain tracer travel time data at different elevations in the study aquifer. This changes the objective of the tests from attempting to determine a number for the so-called full aquifer longitudinal dispersivity α_L^* (which we believe is rather meaningless at the scale of practical tracer tests) to one of gathering information about the advection pattern in the aquifer, which in most situations will dominate the early tracer dispersion process as illustrated in Figure 1. (Field evidence in support of this statement will be presented later.) Because of the emphasis on obtaining accurate tracer travel times at isolated elevations in

the study aquifer, it is vital that multilevel sampling wells be constructed so that dependable data are obtained. Unfortunately, a satisfactory solution to the multilevel sampling well construction problem is not yet available.

Shown in Figure 5 are three multilevel sampling well types. In recent tracer tests with which the authors are concerned, various versions of type I have been attempted. Type I and related types have appeal because of the convenient vertical location of the sampling zones, and the potential economy of installation. Illustrated in Figure 6 is the multilevel sampling system described by Pickens et al. (1978) and later used in single- and two-well tracer tests (Pickens and Grisak, 1981). The system was designed for shallow water table applications and was usually forced into position using a high pressure water jet (Pickens et al., 1978). Identical or similar systems have been utilized or tested by other research groups (Stanford University, Tennessee Valley Authority, personal communications). For the Pickens et al. (1978) system to perform acceptably, the study aquifer must collapse around the sampler and make good contact so that spurious high vertical permeability pathways are not created along or near the aquifer-sampler boundary (Fig. 14). Apparently, this was not a problem in the clean sandy aquifer studied by Pickens and Grisak (1981). However, in more cohesive aquifers with lower vertical hydraulic conductivities and higher vertical head gradients, problems have been observed (Tennessee Valley Authority, personal communication).

Moltyaner and Killey (1986) have developed an automated multilevel sampling system designed for use with radioactive tracers. This system, which uses a dry access well monitoring technique, is illustrated in Figure 7. With this arrangement Moltyaner and Killey (1986) made the equivalent of

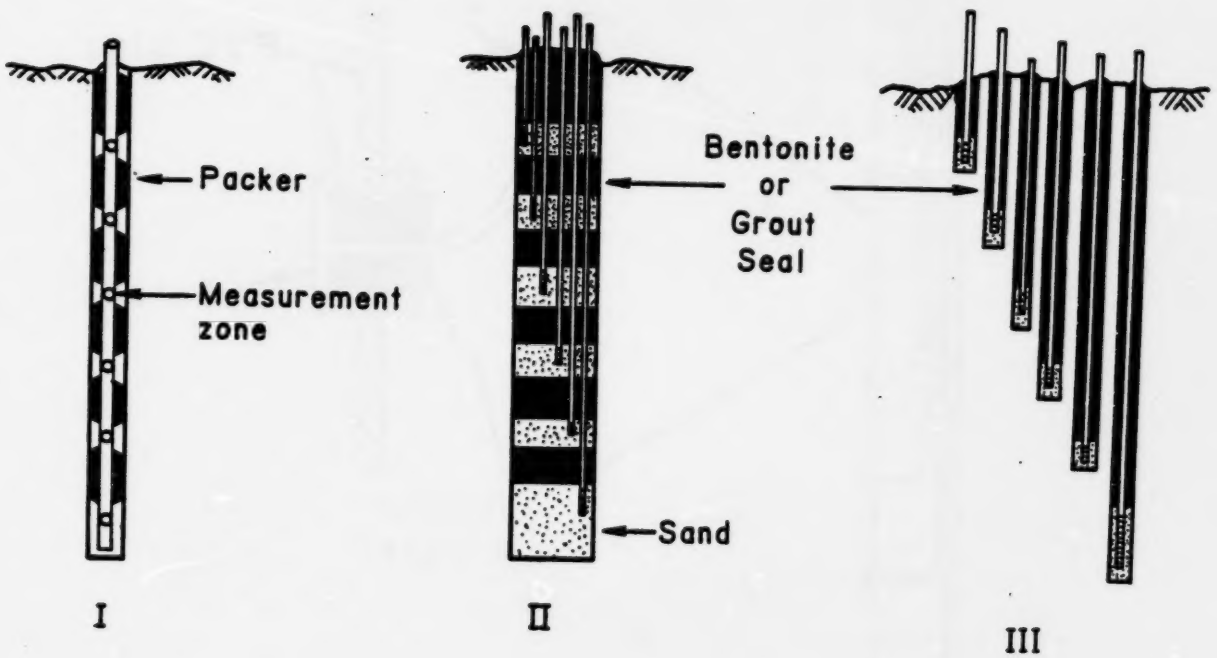

Figure 5. Various types of multilevel sampling systems.

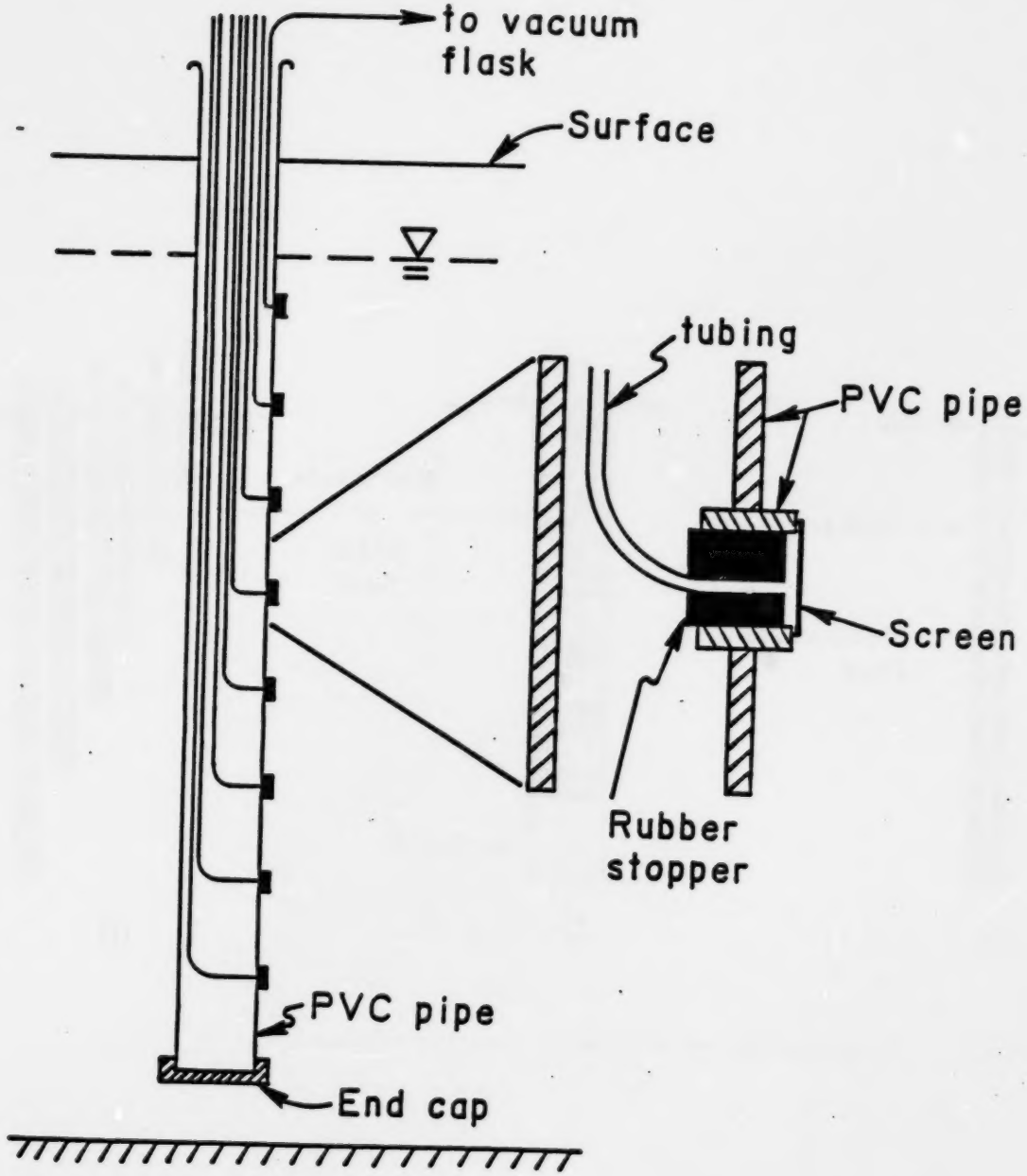

Figure 6. Pickens et al. multi-level sampling/observation well.

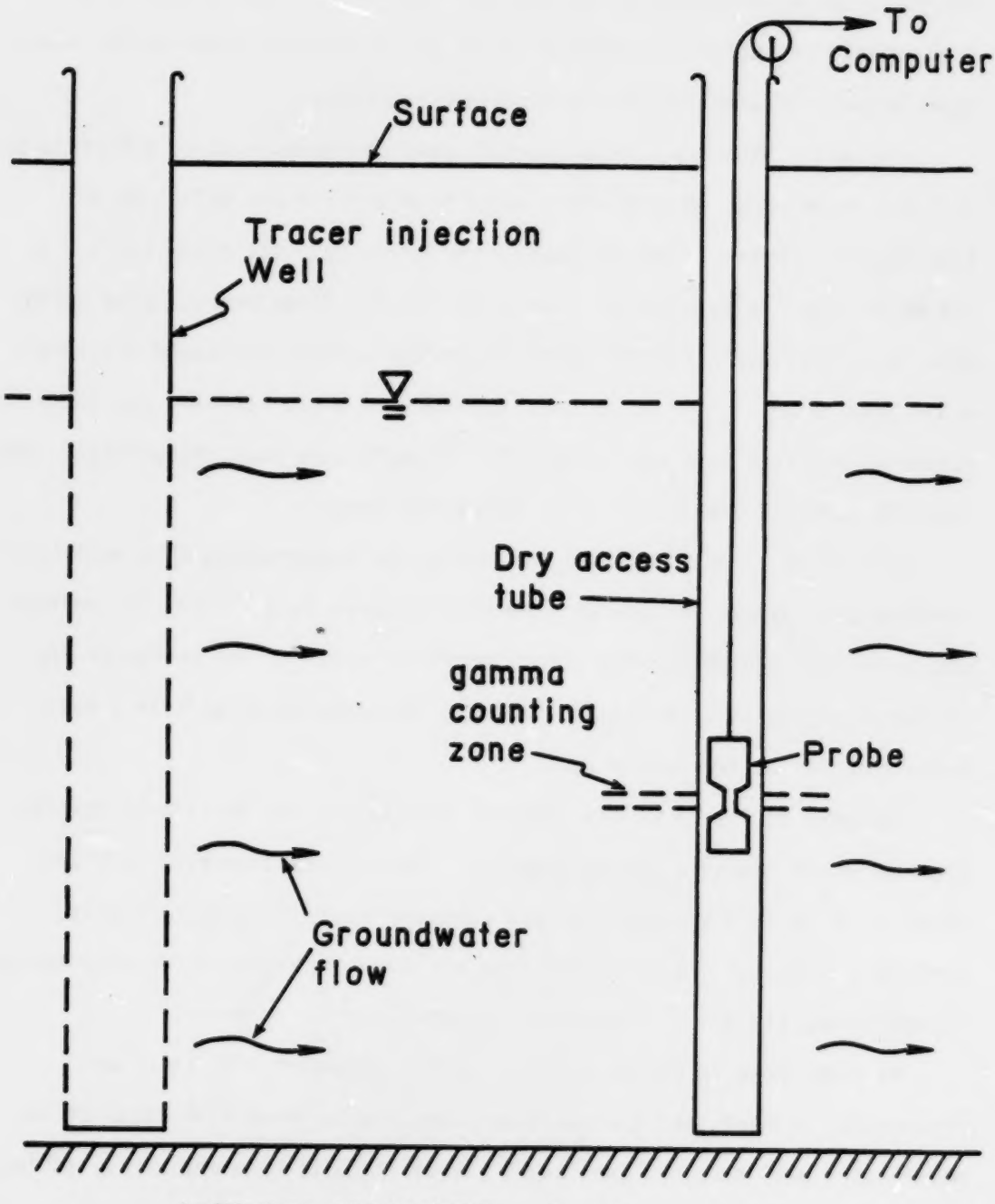

Figure 7. Moltyaner and Killey multilevel, dry, access tube system for use with radioactive tracers.

750,000 point measurements using computer-controlled probe placement and data aquisition, which illustrates one of the tremendous labor-saving advantages associated with the use of radioactive tracers.

Presumably, the dry access tube(s) could be implaced using a variety of drilling techniques, each of which would have a different effect on the tube-aquifer boundary. If the tubes were jetted into the study aquifer or placed in auger holes with the idea of having the formation collapse around them, then the same potential vertical leakage problem discussed previously would seem to exist. If thick drilling mud were used, however, and the access tube placed in a mud-lined hole, it would seem that the potential for spurious vertical leakage would be diminished greatly.

Molz et al. (1985) describe the design and construction of a multilevel sampling well system for use with chemical tracers in a variety of confined and unconfined aquifers. The actual sampling system is not perfected and should be viewed as a prototype. However, it appeared to work in a satisfactory manner at the Mobile site.

As shown in Figure 8, the screened portions of the multilevel observation wells are not of a standard design. The screens themselves are composed of 91 cm (3') slotted sections alternating with 213 cm (7') solid sections. Although 5 slotted sections are shown in Figure 8 for purposes of illustration, the actual screens contained 7 slotted sections.

As also shown in Figure 8, a 5.1 cm (2") diameter PVC insert was constructed with slotted and solid portions that matched with those of the observation well screen. The insert was designed to hold any wires, tubing, or instrumentation that ultimately would be placed in an observation well. Composed of threaded 3.05 m (10') sections, the inserts extended all the way to the land surface. In order to isolate the various sampling zones, the

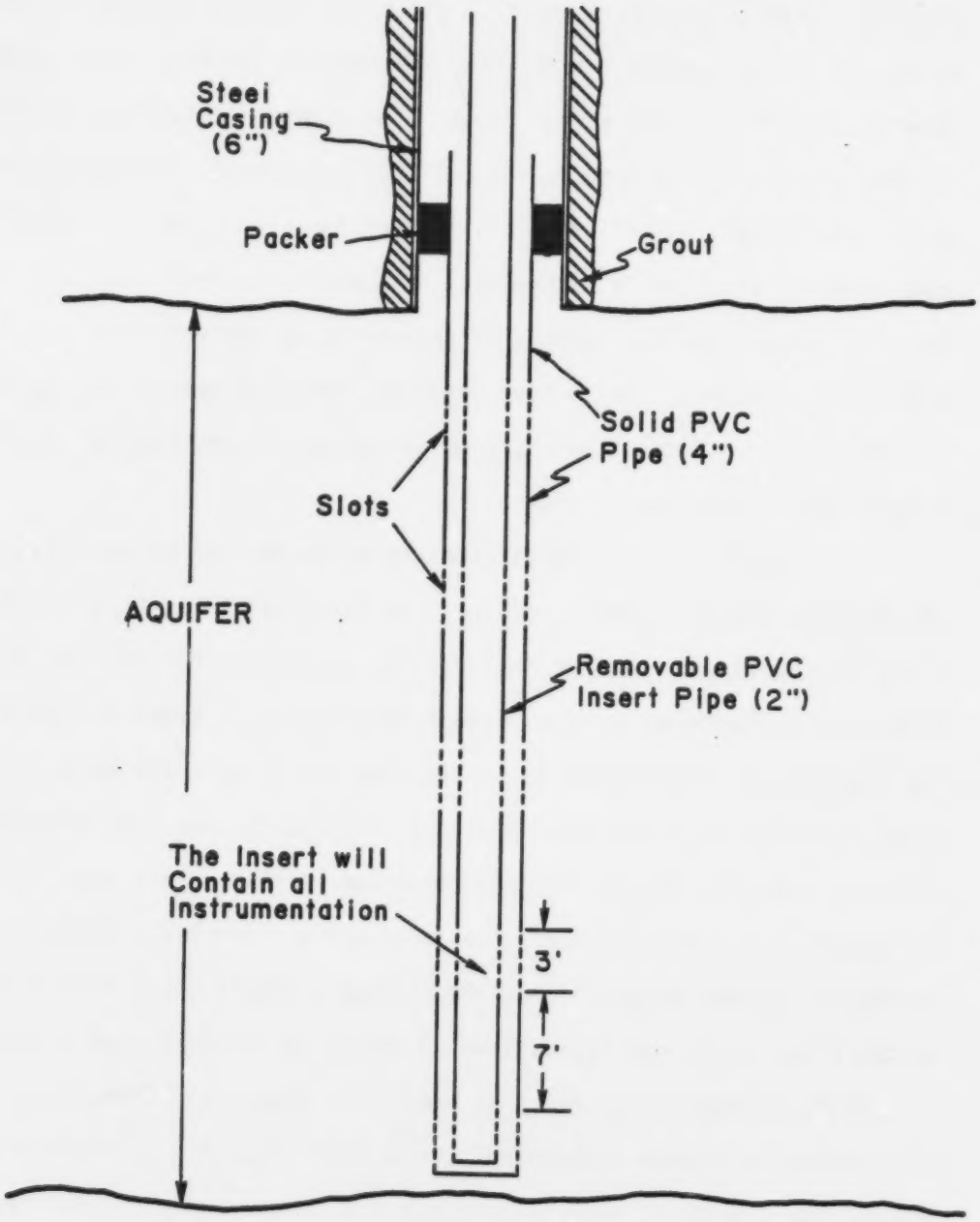

Figure 8. Schematic diagram of the basic construction plan for a multilevel sampling well with a removable insert.

inserts were fitted externally with cylindrical annular inflatable packers as illustrated in Figures 9 and 10. After the required probes, tubing and wires were placed within the inserts, the sampling sections were isolated internally with silicone rubber plugs. The complete insert was constructed on the surface, then placed in the well, using a crane, positioned and the packers inflated. After installation, each isolated 91 cm (3') sampling zone appeared as shown in Figure 11. A conductivity probe was placed near the zone center, and two lengths of vacuum tubing connected the sampling zone to the surface. This tubing could be used with peristaltic pumps to mix the contents of the sampling zone and to obtain groundwater samples for analysis as illustrated in Figure 12.

In designing the multilevel sampling wells for use at the Mobile site, the drilling and well development process illustrated in Figure 13a,b was visualized. After removal of the drilling equipment, the drilling mud and disturbed aquifer material are mixed significantly as shown in Figure 13a. The cleaning and development procedure then was to pump and surge the wells until the water was clear and devoid of drilling mud and fine material. As shown in case (b), Figure 13, this procedure probably left some drilling mud adjacent to the solid casing segments and a disturbed (perhaps more permeable) aquifer material near the slotted segments where samples were to be collected. Such mud remnants would not be left behind (see Figure 13c) if a fully slotted screen had been used. The potentially beneficial effects of a partially slotted (segmented) screen with respect to a fully slotted screen, and a vertical leakage path possible in the fully slotted case, are illustrated further in Figure 14. The drilling mud remnant adjacent to the solid portion of the screen may result in a barrier to vertical flow that is very desirable. For the fully slotted screen, very little mud remains after

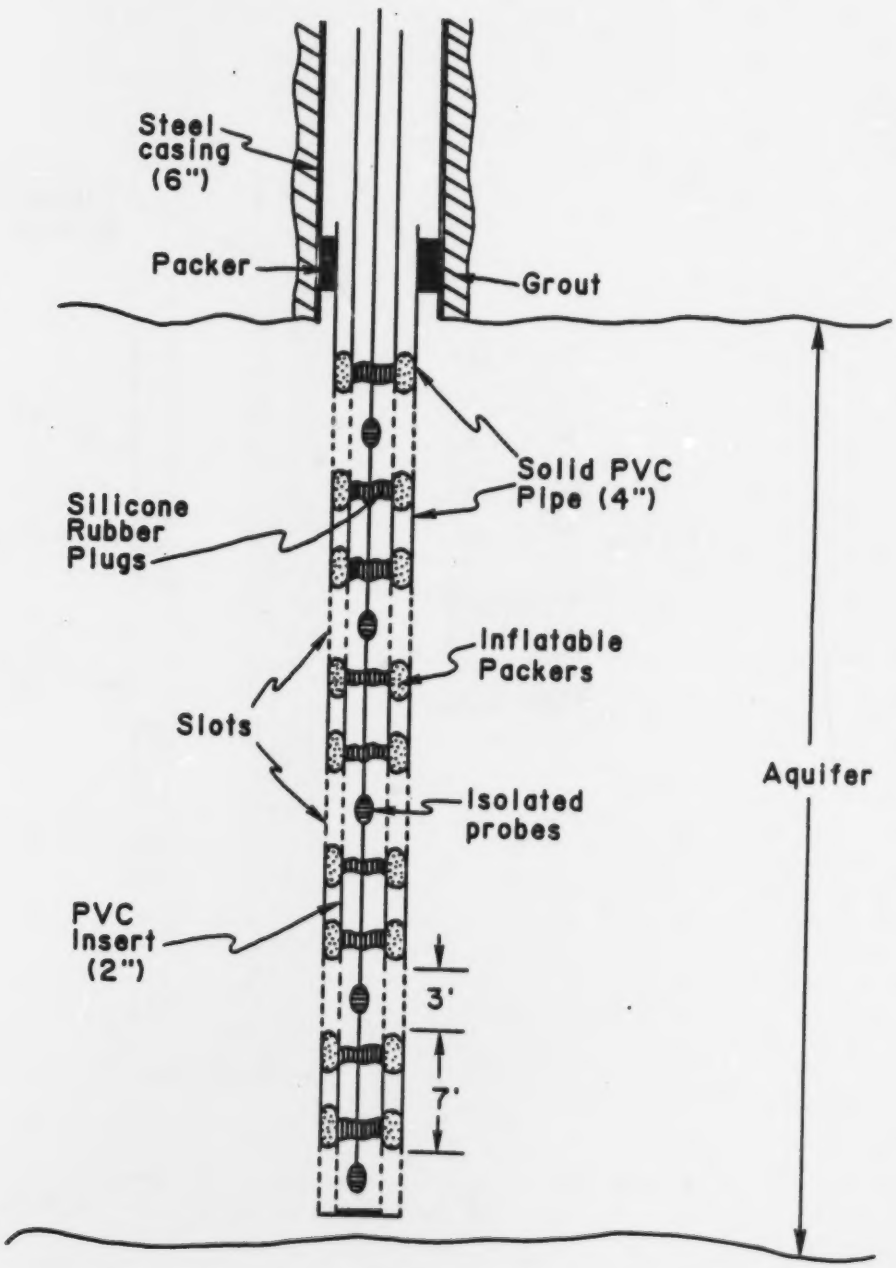

Figure 9. Multilevel sampling well with sampling zones isolated with inflatable packers and silicone rubber plugs.

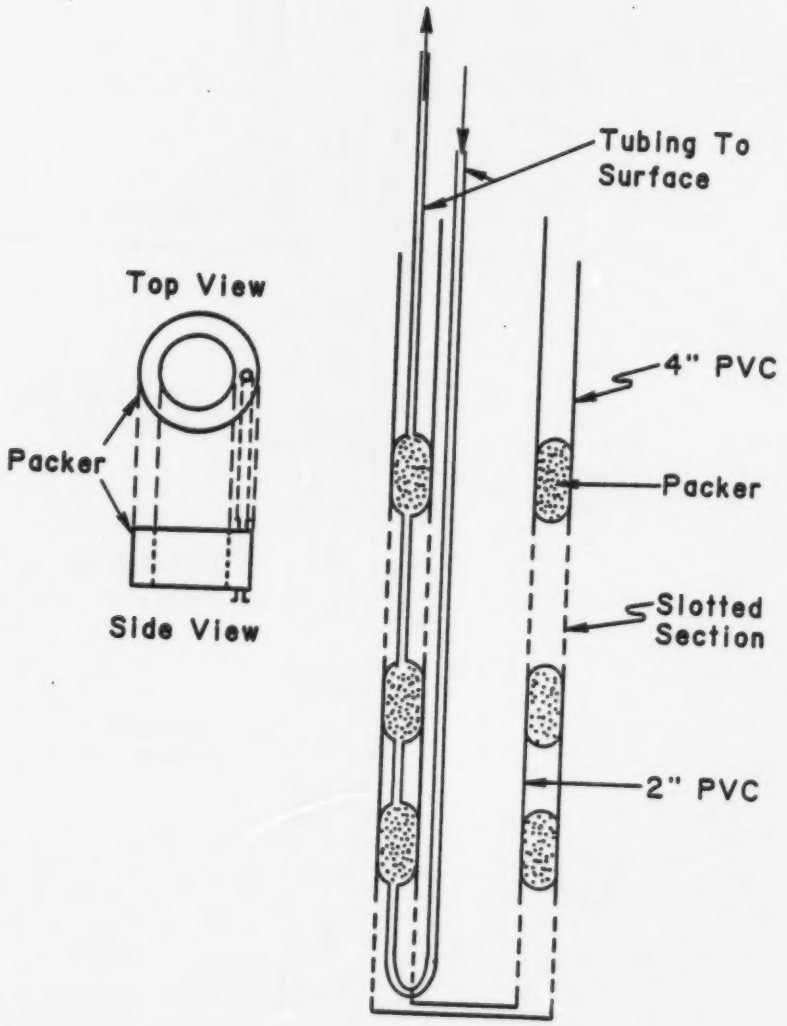

Figure 10. Details concerning the geometry and installation of inflatable packers. The packers were inflated with water.

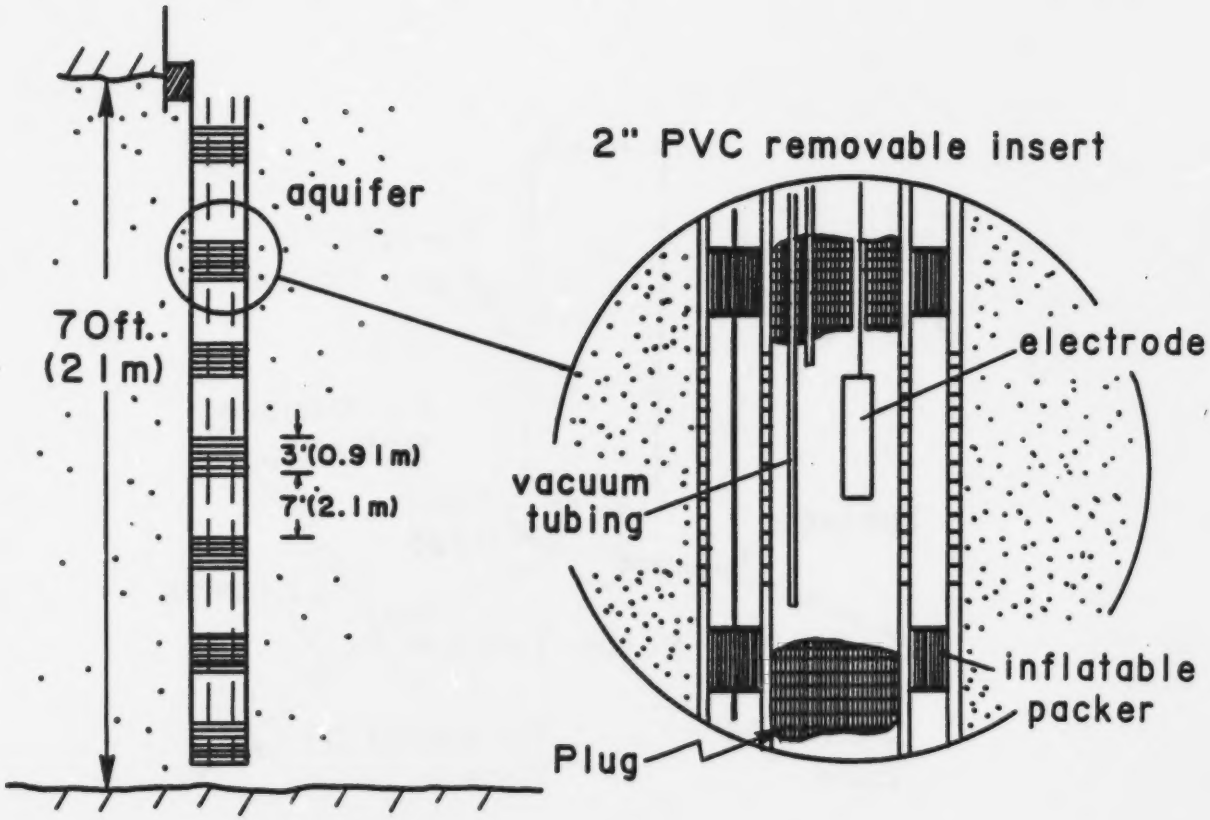

Figure 11. Diagram of a completed multilevel sampling well. This and similar systems were used at the Mobile site.

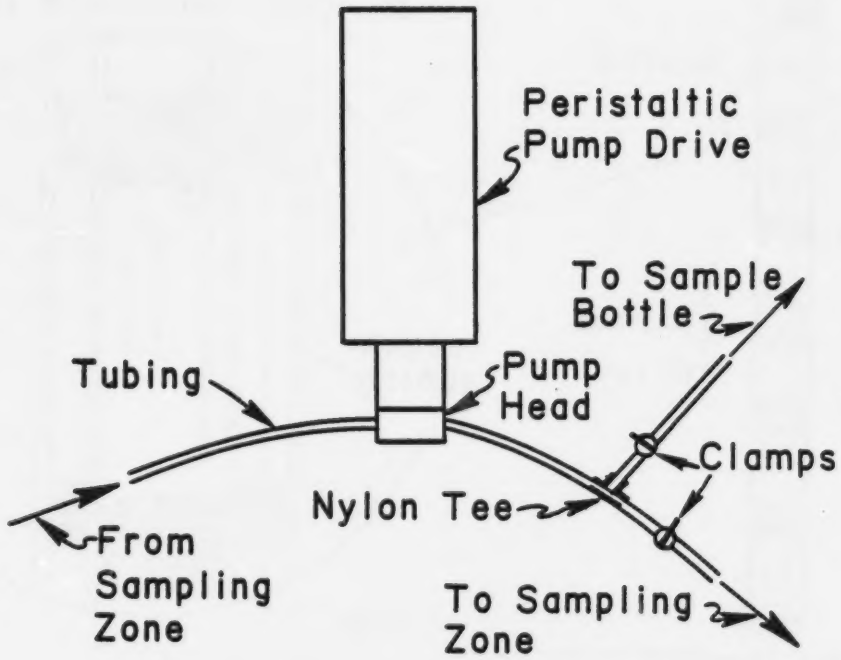

Figure 12. Diagram illustrating the scheme for causing mixing in the various isolated sampling zones and obtaining samples for laboratory analysis.

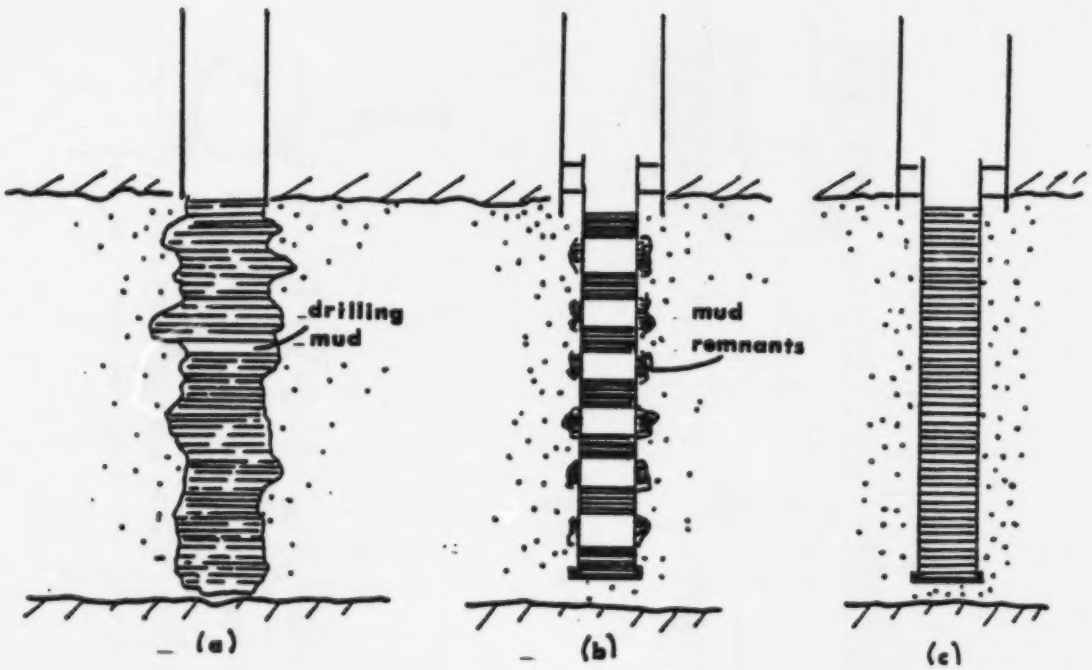

Figure 13. Diagram illustrating what may happen during drilling and installation of various types of screens.

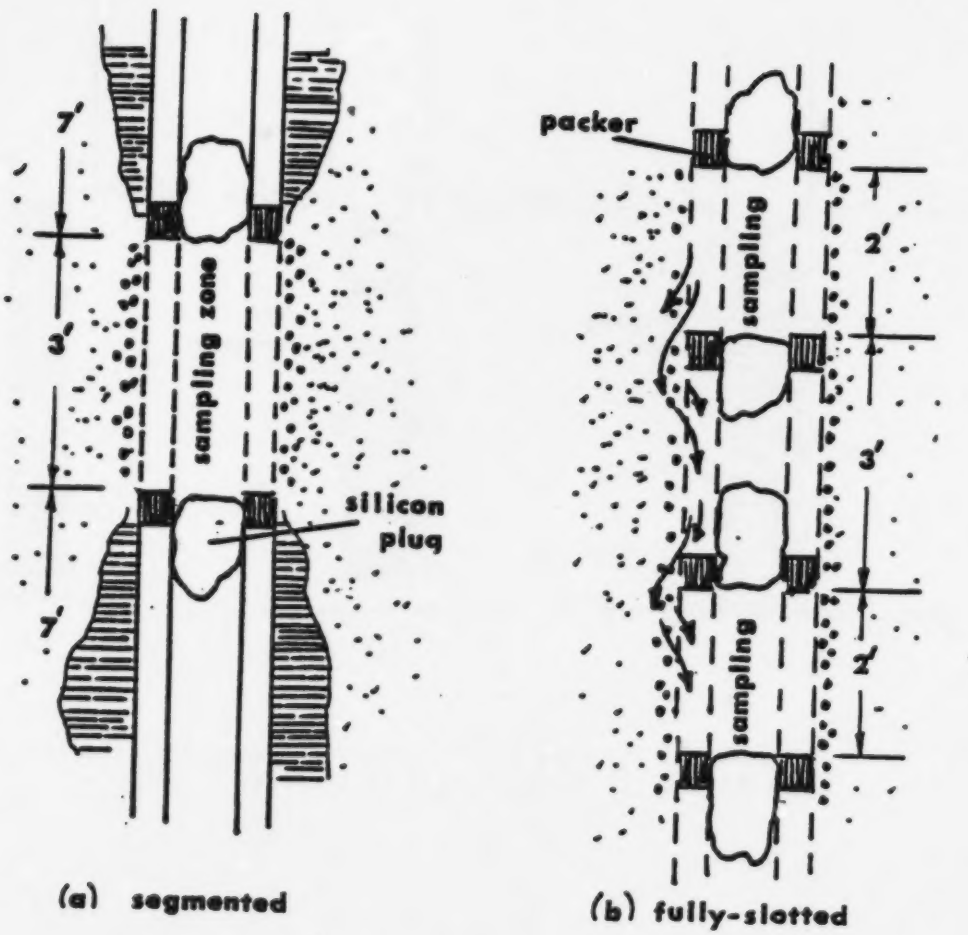

Figure 14. Details concerning the possible beneficial effects of drilling mud left behind in the formation (a) and possible leakage paths associated with fully-slotted screen (b).

development and a disturbed aquifer material of possibly higher permeability would result along the entire length of screen.

The most thought out and best designed multilevel sampling system from a vertical integrity viewpoint of which the authors are aware appears to be the multiple port system manufactured by Westbay Instruments, Ltd. of Vancouver, B.C. In its present configuration, however, the system is suited for groundwater monitoring but not tracer testing which requires the ability to sample rapidly and simultaneously from a number of elevations. Lack of a solution to the vertical integrity problem valid in a broad range of aquifer types coupled with the unavailability of economic, dependable and flexible commercial equipment is a major impediment to the practical application of most types of multilevel tracer testing.

Performance and Results of Single-Well and Two-Well Tracer Tests at the Mobile Site

Using the multilevel sampling wells described in the previous section, a series of single-well and two-well tracer tests were performed at the Mobile site over the past two years. The major purpose of these tests was to measure the tracer travel times between an injection well and one or more multilevel sampling wells. Subject to several assumptions to be discussed later in this section, the resulting travel time data allows one to infer a vertical distribution of horizontal hydraulic conductivity. We view the experiments to be described as the simplest and most convenient tracer tests which yield some information about the variation of aquifer hydraulic properties with respect to the vertical position in the aquifer. The basic experimental plan was to conduct a series of single-well and two-well tests at different locations in an attempt to build up a three-dimensional picture of the hydraulic conductivity distribution. We did not attempt to make point measurements or nearly point measurements as was done by Pickens and

Grisak (1981). Our objective was to average tracer travel times over a suitable aquifer thickness. Thus the inferred hydraulic conductivity distribution that results may be viewed as being based on a type of spatial average.

The project site is located in a soil borrow area at the Barry Steam Plant of the Alabama Power Company, about 32 km (20 mi) north of Mobile, Alabama. The surface zone is composed of a low-terrace deposit of Quaternary age consisting of interbedded sands and clays that have, in geologic time, been recently deposited along the western edge of the Mobile River. These sand and clay deposits extend to a depth of approximately 61 m (200 ft) where the contact between the Tertiary and Quaternary geologic eras is located. Below the contact, deposits of the Miocene series are found that consist of undifferentiated sands, silty clays and thin-bedded limestones extending to an approximate depth of 305 m (1000 ft). The study formation is a confined aquifer approximately 21 m (69 ft) thick which rests on the Tertiary-Quaternarty contact.

Except for the well diameters, Figure 15 is a vertical section scale drawing of the subsurface hydrologic system at the Mobile site. Included in the drawing are 3 pumping wells (E1, I2 and E10) and 4 multilevel observation wells (E5, E3, E7 and E9) all situated at approximately the same vertical plane. (A schematic plan view showing the wells E1 and I2 and the supply well S2 is given in Figure 17). The study aquifer is well confined above and below by clay-bearing strata that probably extend laterally for several thousand feet or more, and the natural piezometric surface of the confined aquifer at the test site is at a depth of 2 to 3 m (6 to 10 ft) below the ground surface. In experiments performed to date, vertical hydraulic gradients within the aquifer have been small. A medium to fine

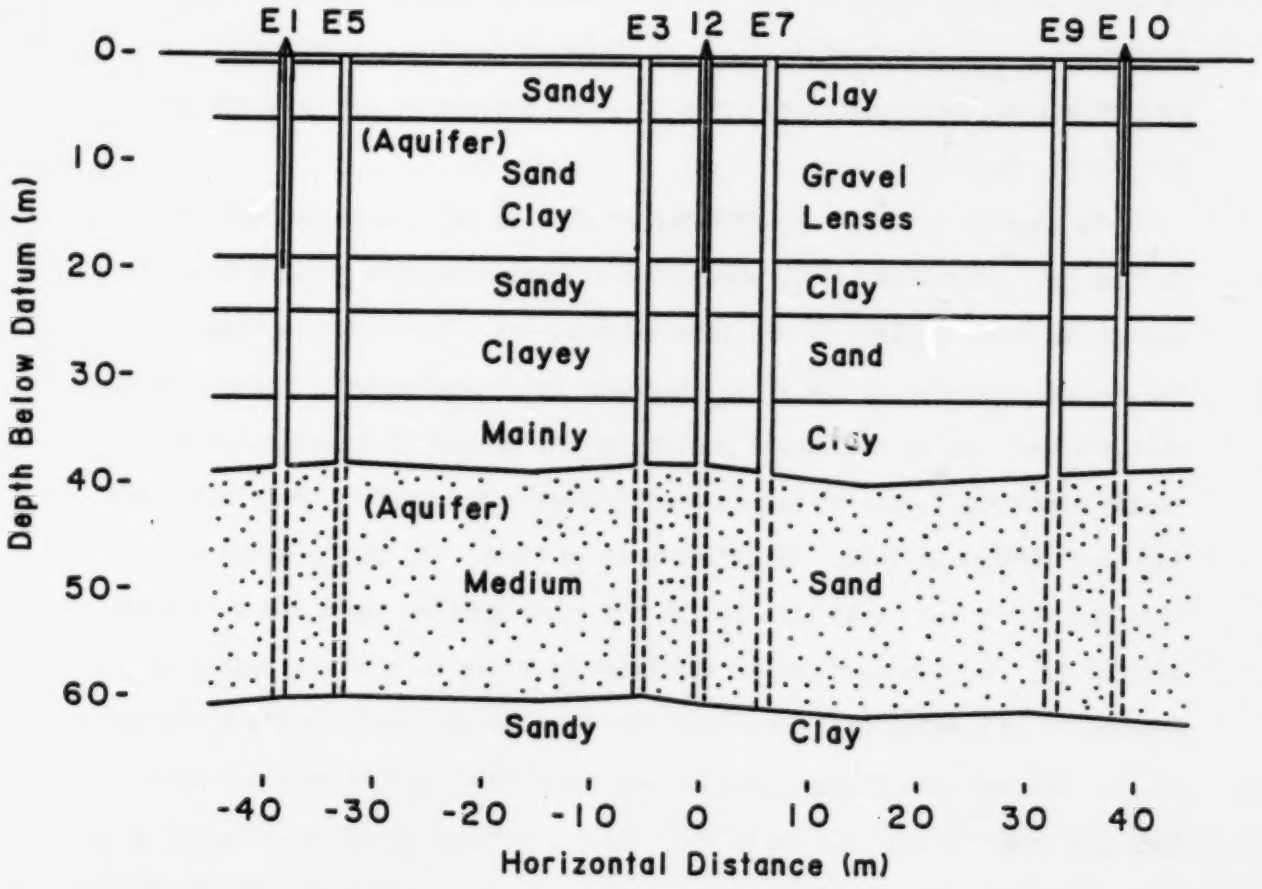

Figure 15. Diagram of the subsurface hydrologic system at the Mobile site where tracer tests were performed. Wells E1, I2 and E10 are pumping wells, while E5, E3, E7 and E9 are multilevel sampling wells. All wells shown are situated at approximately the same vertical plane. See Figure 17 for a schematic plan view showing wells E1 and I2.

sand containing approximately 3 percent silt and clay by weight composes the main aquifer matrix at well E3. (At other locations in the aquifer the fines vary from 1% to 15% by weight.) When E3 was constructed, moderately disturbed cores were obtained at 7 locations throughout the depth of the study aquifer using a Shelby tube. The resulting particle size and distribution data, which we believe are accurate despite the moderate disturbance, are presented in Table 1. Further details concerning aquifer/aquitard hydraulic and other physical properties may be found in Parr et al. (1983).

The pumping wells are constructed of 20.3 cm (8") steel casings with 15.2 cm (6") stainless steel, wire wrapped screens and are grouted from the top of the study aquifer to the land surface. As illustrated in Figure 16, the piping and valve system associated with each pumping well is designed so that the well can be used for injection or withdrawal of tracer solution. In the single-well test to be reported in detail herein, tracer solution was injected through well I2. As illustrated in Figure 17, supply water was obtained from a well (S2) screened in the study aquifer about 244 m (800 ft) east of I2. This separation was sufficiently large so that the hydraulic effects of S2 pumping did not affect the tracer experiments in the vicinity of I2. Concentrated tracer solution was mixed in a 4800 liter (1270 gal) tank and added to the 10.2 cm (4 in) pipeline connecting S2 and I2 using a metering pump. The pipeline travel distance from the metering pump to the study aquifer was at least 160 m (525 ft) which was more than sufficient to insure complete mixing of the tracer. It was assumed that the piezometric head distribution in the injection well screen was uniform with depth since the screen diameter was 15.2 cm (6 in) which resulted in a maximum average vertical fluid velocity in the screen of 0.84 m/s (2.75 ft/s) (during

Table 1. Particle size distribution data for the seven disturbed cores obtained during construction of well E3.

Depth of Core (m)	D_{60} (mm)	D_{30} (mm)	D_{10} (mm)	Percent Passing #200 Sieve (%)
40.2	0.46	0.35	0.21	1.8
43.3	0.36	0.26	0.13	1.4
46.6	0.58	0.45	0.21	3.0
49.7	0.46	0.27	0.12	5.6
52.7	0.49	0.28	0.15	3.5
56.1	0.59	0.44	0.26	1.2
59.1	0.94	0.56	0.19	3.8

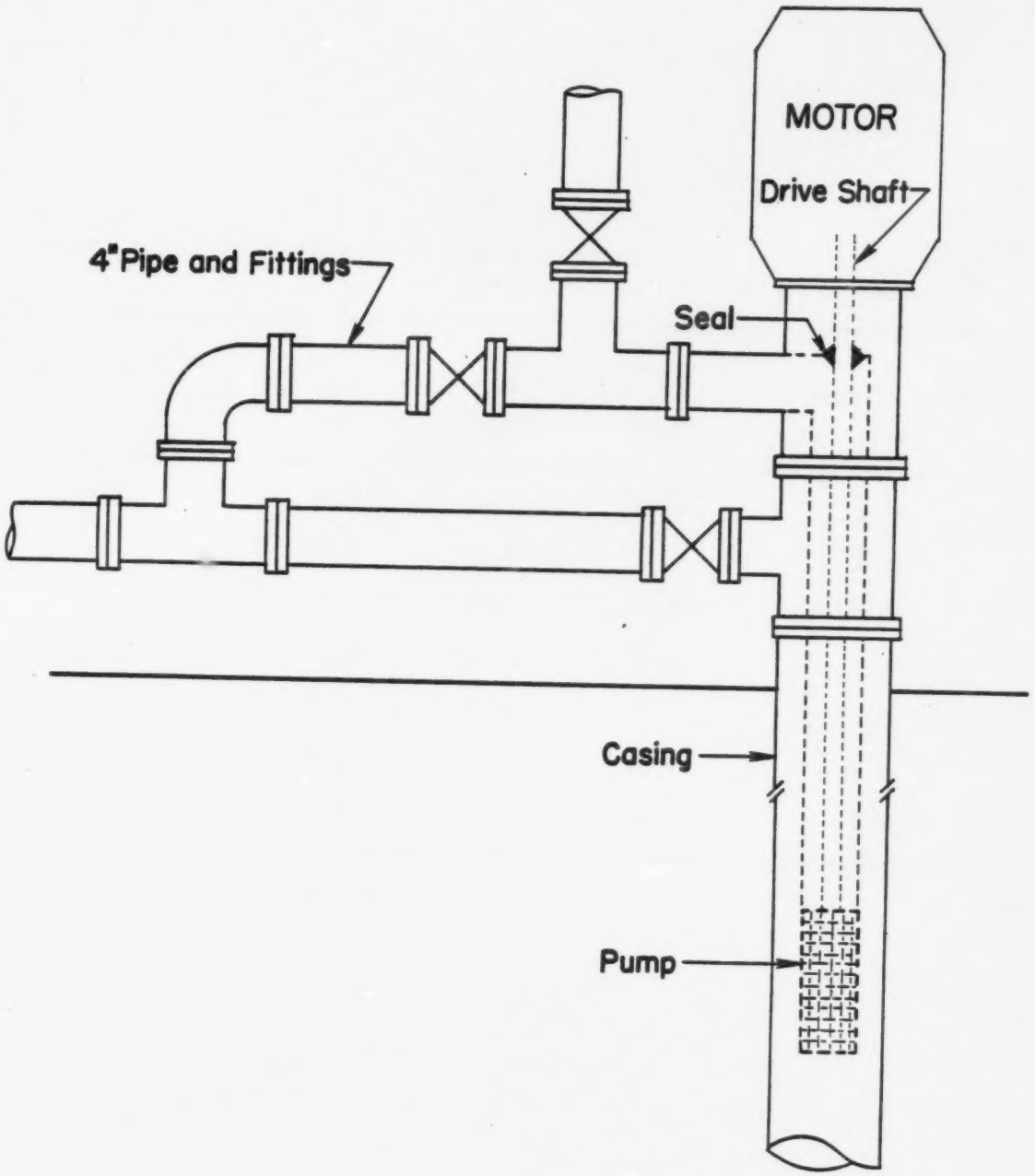

Figure 16. Piping and valving scheme associated with pumping wells at the Mobile site.

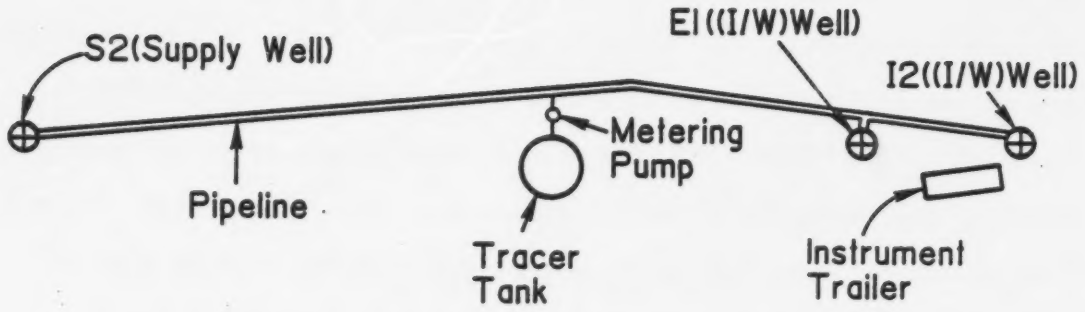

Figure 17. Diagram showing the main features of the surface hydraulic system used in the single- and two-well tracer tests at the Mobile site.

experiment #4). Thus the maximum velocity head was only 0.037 m (0.12 ft) and the head losses due to friction along the 21 m (69 ft) length of screen would be less than 0.10 m (0.33 ft). These totals when compared to the injection head of approximately 3 m (9.8 ft) are consistent with the assumption of constant head in the well screen interior.

As discussed in detail by Molz et al. (1985), several preliminary tests were conducted with the objective of assessing the vertical integrity of the multilevel sampling wells and the effect of mixing the water within each sampling zone which was approximately 0.91 m (3 ft) high. It was concluded that sample zone isolation was adequate for tests which were to follow. There was a significant difference between breakthrough curves at the seven sampling zones depending on whether sample zone mixing was induced. Therefore, it was concluded that mixing within each isolated sampling zone is desirable. For a sampling zone of finite length it is possible for the tracer to enter the zone anywhere along the slotted length and then be recorded depending on unknown natural mixing and probe position. Imposed mixing forces an integration effect causing tracer concentration to be more representative of the entire length of the sampling zone. (This relates back to the moving average concept discussed previously.) Without imposed mixing, the effective sampling length in the vertical direction is unknown.

Single-Well Test

The first complete single-well tracer test conducted at the Mobile site was labeled "experiment #4" and utilized the multilevel sampling well E3 (Figure 15). To start the experiment, supply groundwater without tracer was injected into I2 until the initial transients disappeared and a steady injection rate resulted (approximately 2 hours). Then at time zero tracer was added to the injection water, and the actual test initiated. Shown in

Figure 18 are the bromide concentrations measured in I2 (injection/withdrawal well), while the concentration breakthrough curves measured in E3 (multilevel sampling well) are shown in Figure 19. (Water samples were obtained from the injection/withdrawal well using a faucet in the pipeline.) During the experiment tracer solution at an average concentration of 242 mg/l was injected at the rate of 0.915 m^3/min (242 gpm) for the first 32 hours. This injection rate, without tracer added to the water, was maintained for the next 22 hours at which time injection was halted. One hour and 15 minutes later withdrawal pumping was initiated at the rate of 1.19 m^3/min (314 gpm) and continued for two weeks so that virtually all tracer was removed from the system. Note that Figure 18 contains both injection and withdrawal data while Figure 19 contains only injection breakthrough data.

Table 2 contains the time for 50% of breakthrough for each level based on the electrical conductivity measurements for experiment #4 shown in Figure 20 and the concentration data shown in Figure 19. With the probable exception of level 1, the concentration data look quite good. On the average, the arrival times based on electrical conductivity lag those based on concentration by about 2 hours. (We will refer to this as the "two-hour rule" later on.) This is largely due to the fact that the electrical conductivity of the supply water, which is ultimately mixed with tracer, is lower than that of the native groundwater in the vicinity of I2 by about 16%, caused in part by water chemistry changes induced by previous aquifer thermal energy storage experiments at the same site (Molz et al., 1983). Thus as the tracer solution approaches a conductivity probe, the reading will decrease initially even though the bromide concentration is increasing. The net effect of this interaction is to cause the electrical conductivity

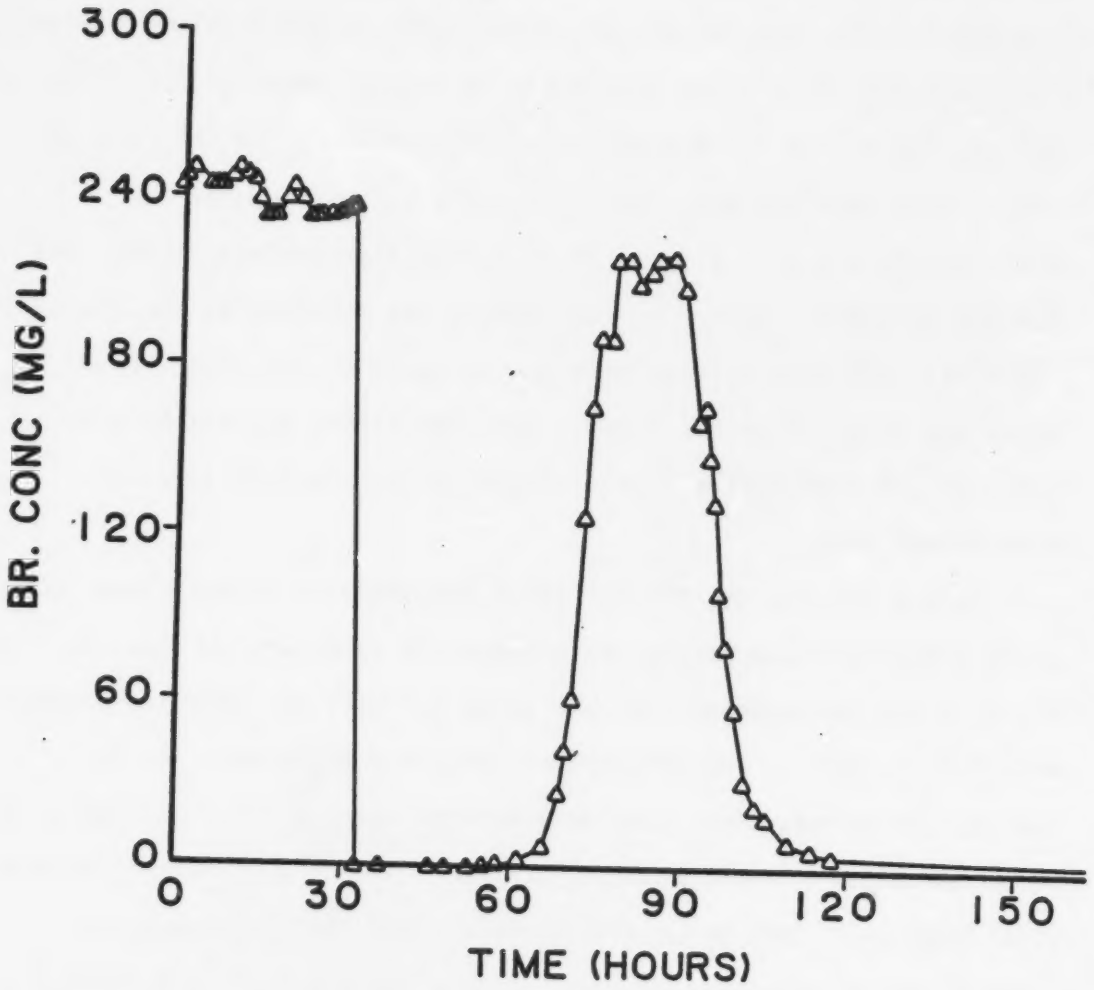

Figure 18. Bromide concentration in the injection/withdrawal well (I2) during experiment #4. Tracer injection ended at t=32 hours; injection ended at t=54 hours. Withdrawal began at t=55.25 hours.

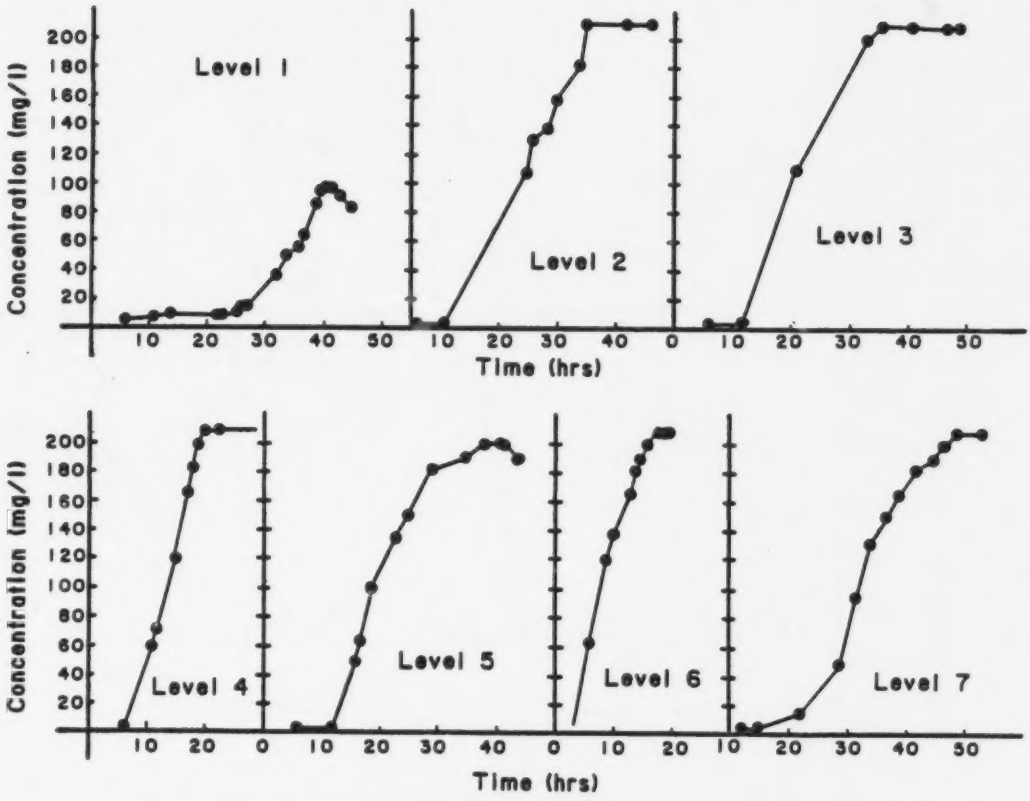

Figure 19. Bromide concentration breakthrough curves at the seven levels of well E3 during experiment #4.

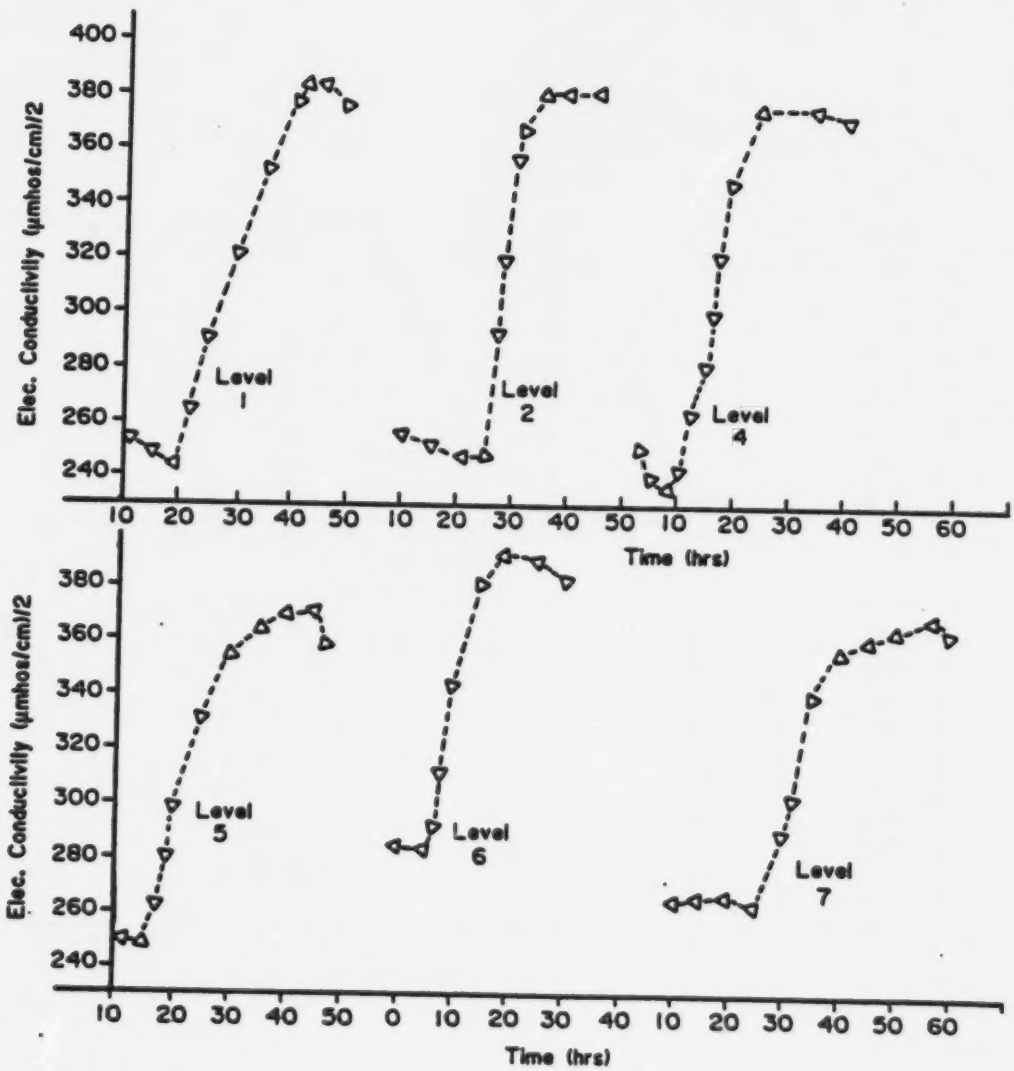

Figure 20. Electrical conductivity breakthrough curves at various levels of well E3 during experiment #4.

Table 2. Sampling zone elevations, arrival times for fifty percent breakthrough, apparent dispersivity values and inferred normalized hydraulic conductivity values for experiment #4.

Level #	Mid-Zone Elevation	Arrival Times from Concentration Measurements	Normalized Hydraulic Conductivity	Apparent Dispersivity	Arrival times from Electrical Conductivity Measurements	Normalized Hydraulic Conductivity
1	-40.7 m	33.4 hr?	0.24	0.07±0.01 m	29.0 hr	0.34
2	-43.8 m	24.3 hr	0.33	0.18±0.02 m	27.3 hr	0.37
3	-46.8 m	20.5 hr	0.39	0.17±0.06 m	--	--
4	-49.9 m	14.0 hr	0.57	0.12±0.04 m	16.0 hr	0.63
5	-52.9 m	19.0 hr	0.44	0.32±0.08 m	21.8 hr	0.46
6	-56.0 m	8.0 hr	1.00	0.50±0.03 m	10.0 hr	1.00
7	-59.0 m	32.4 hr	0.25	0.04±0.01 m	33.2 hr	0.30

data to overestimate the actual mid-rise arrival time. Presumably, this could be corrected by adding additional ions, other than bromide, to the supply water. However, we did not attempt this because the probe recordings were used mainly to orient ourselves qualitatively as to what was happening in the subsurface. Ultimately, calculations of normalized hydraulic conductivity were based mainly on arrival times deduced from concentration data measured in the laboratory. The results of both are shown in Table 2 mainly for comparison and information purposes.

Tracer travel time data alone does not enable one to calculate an absolute value of hydraulic conductivity. To calculate such a value for the general nonhomogeneous case, one must know the flow path, porosity and hydraulic head distribution along the flow path in addition to the travel time. It was not feasible to measure all these quantities during our tracer tests. However, if one approximates the real aquifer in the test vicinity with a perfectly stratified aquifer of constant porosity and horizontal layering, then for a fully penetrating injection well the Darcy velocity at the elevation of each sampling zone will be horizontal and proportional to the hydraulic conductivity at that level. Thus the following equations can be written

$$K_i = \beta(R)v_i(R) = \frac{1}{2}\beta(R)R/t_i = \frac{\pi\theta TR^2}{Qt_i} \qquad (6)$$

where K_i = horizontal hydraulic conductivity at the ith level, $\beta(R) = \theta/(dh/dr)$ where θ is the porosity and dh/dr is the hydraulic gradient at radius R, v_i = seepage velocity at the ith level, R = constant radial distance between the injection well and a particular multilevel sampling well, t_i = tracer travel time between the two wells at the ith level, T =

aquifer transmissivity, and Q = injection flowrate. At any particular level, t_i is taken as the time between the start of tracer injection and when 50% of breakthrough occurs. In any given experiment there will be a minimum arrival time, t_{min}, which corresponds to the layer with the largest hydraulic conductivity, K_{max}, and from equation (6)

$$K_{max} = \frac{1}{2} \beta(R) R / t_{min} \tag{7}$$

Forming the ratio of equations (6) and (7), one arrives at what can be called the normalized hydraulic conductivity

$$\frac{K_i}{K_{max}} = \frac{t_{min}}{t_i} \tag{8}$$

It is also possible to calculate the ratio $K_i/\bar{K} = \bar{t}/t_i$, where the "bar" notation indicates average values (Pickens and Grisak, 1981). $\bar{K}$ could then be equated, as a first approximation, to the hydraulic conductivity obtained from a fully penetrating pumping test, as $\bar{K} = T/B$ where T is the transmissivity and B is the aquifer thickness. This would enable explicit values to be calculated for each K_i.

We would like to re-emphasize that the simple equations (6) through (8) all result from the "stratified aquifer" approximation which many hydrologists may consider too idealized to represent a real aquifer. There is certainly some merit to this viewpoint. However, the only other practical alternative that we see at the present time is to make the usual assumption of a homogeneous or statistically homogeneous aquifer and go after a full-aquifer dispersivity which, as discussed in the introduction, is a much worse approximation. More will be said about this later.

Based on equation (8), Figure 21 resulted which is a plot of normalized hydraulic conductivity (K/K_{max}) as determined from the concentration data of experiment #4. Since the concentration data for level 1 are not consistent with that from the other levels (perhaps a tubing leak?), we used the electrical conductivity data and the 2-hour rule (see page 22) to provide an improved estimate of the level 1 relative permeability. At this level the electrical conductivity data were normal in appearance and resulted in the level 1 value on the curve shown in Figure 21. The results displayed indicate the presence of a high permeability zone in the bottom third of the aquifer, along the line connecting E3 and I2. This result is consistent with the findings from previous thermal energy storage experiments at the Mobile site which indicated the presence of a high permeability zone, although at a slightly higher elevation in the aquifer (Molz et al., 1983; Buscheck et al., 1983).

In displaying the data of Figure 21, it was decided to simply draw straight lines between the points where hydraulic conductivity was known or measured. In doing this use was made of nine points--the top and bottom of the aquifer, where the clay confining layers force the permeability to essentially zero, and the seven sampling points where tracer travel times were recorded.

Two-Well Test

As described previously, a two-well test may be used with one or more multilevel sampling wells to obtain tracer travel time information similar to that obtained with a single-well test. However, the two-well test is generally performed on a larger scale and, therefore, is more time consuming. At the Mobile site our single-well tests lasted about 5 days, while the two-well tests required 30 to 35 days followed by a month or more

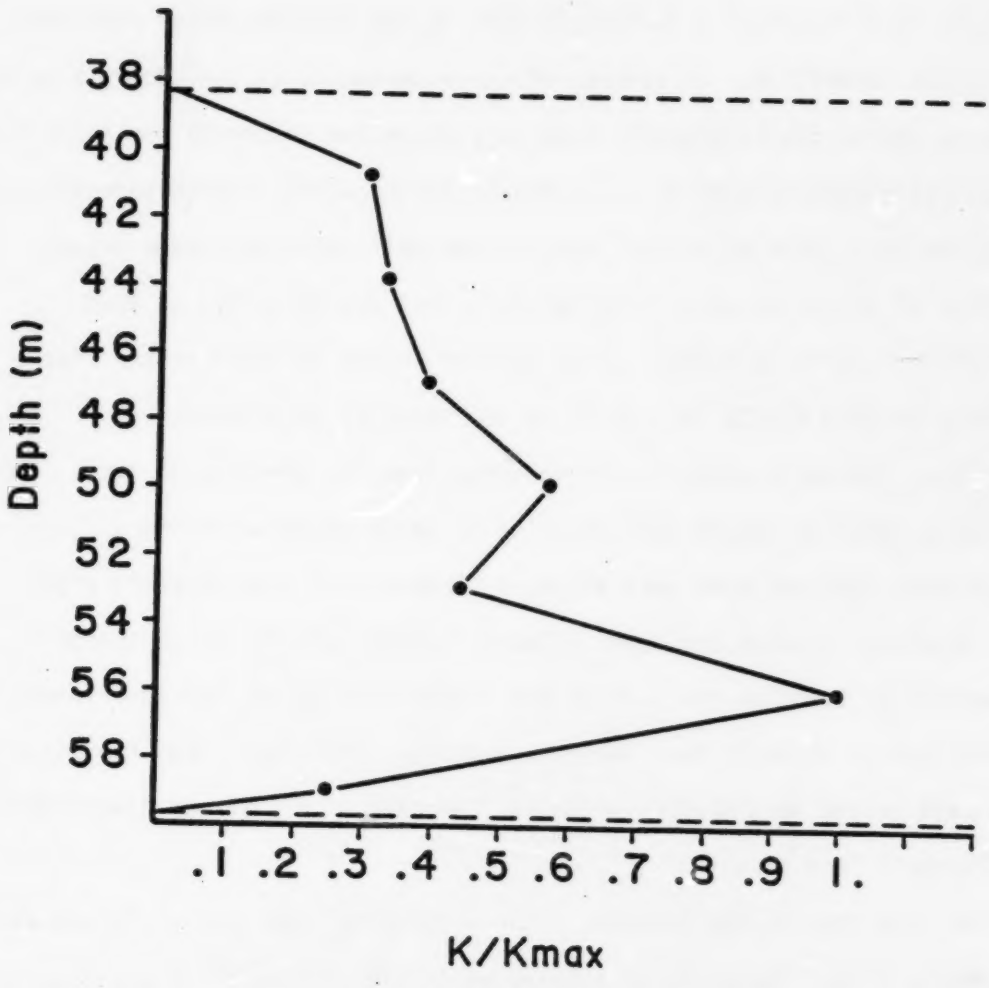

Figure 21. Inferred normalized hydraulic conductivity distribution based on the results of experiment #4 and the stratified aquifer assumption.

of withdrawal to remove all remnants of tracer. Generally speaking, single-well tests are suited for relatively low cost but small scale hydraulic conductivity measurements because only a single pumping well is required. A two-well test in the non-recirculating mode requires at least 2 pumping wells but provides the advantage of being able to move water relatively rapidly over larger travel distances.

Another aspect of a two-well test which was exploited in the present study is that it offers a convenient vehicle for testing tracer transport prediction capability. In several of our experiments at the Mobile site we chose to employ the single-well test as a means for inferring the hydraulic conductivity distribution in a relatively small aquifer region between an injection well and a multilevel observation well (maximum tracer travel distance of 5.5 m (18 ft)). The two-well test was then used to test predictions over a relatively large aquifer region (minimum tracer travel distance of 38.3 m (126 ft)) based on the vertical distribution of horizontal hydraulic conductivity inferred from the single-well test. This procedure helps to define what is actually being measured during a single-well test and over what travel distances such a measurement might have meaning. It also provides valuable insight concerning fundamental properties of the flow field which was established during the experiments. Predictions of two-well test outcomes based on single-well test results are discussed in the next section entitled "Computer Simulation of Single-Well and Two-Well Test Results."

At this time in the project, 2 two-well tests have been performed at the Mobile site. The pairs of pumping wells used in the first and second tests, respectively, were E1-I2 and I2-E10. Both tests were done in the non-recirculating mode with E1 and I2 used as injection wells in the first

test and second test, respectively. Herein, only the E1-I2 test will be described in detail.

Preparation for the execution of a two-well test is similar in philosophy to that for a single-well test. The first step is to establish the flow field between the injection and withdrawal wells using groundwater without tracer. As illustrated in Figure 17, the piping between E1 and I2 was valved off, and a pump in well S2 was used to inject water into E1. Simultaneously, a pump in I2 withdrew water which was then wasted. Discharges were measured with standard turbine-type water meters and only minor valve adjustments were required in order to get the injection and withdrawal rates essentially equal and to maintain equality throughout the test. Following flow field establishment, tracer injection was initiated simply by turning on the metering pump in the line connecting the tracer tank to the S2-E1 pipeline (Fig. 17). The E1-I2 test was performed within the geometry illustrated previously in Figure 15. Both the injection well (E1) and withdrawal well (I2) have 15.2 cm (6") diameter stainless steel screens that fully penetrate the study aquifer. The observation wells (E5 and E3) are constructed of PVC pipe as described in the discussion of multilevel sampling well design and construction.

The test began (tracer injection initiated) at 9:50 AM on August 31, 1984 and continued until 8:00 AM on October 2, 1984. Injection and withdrawal rates averaged 0.946 m^3/min (250 gpm) and, typically, were equal to within less than 1%. Tracer was added to the injection water during the first 76.6 hours of the experiment which resulted in the injection concentration versus time function shown in Figure 22. After approximately 70 hours, tracer began to appear in the withdrawal well. As shown in Figure 23, the withdrawal concentration versus time function was complex, and

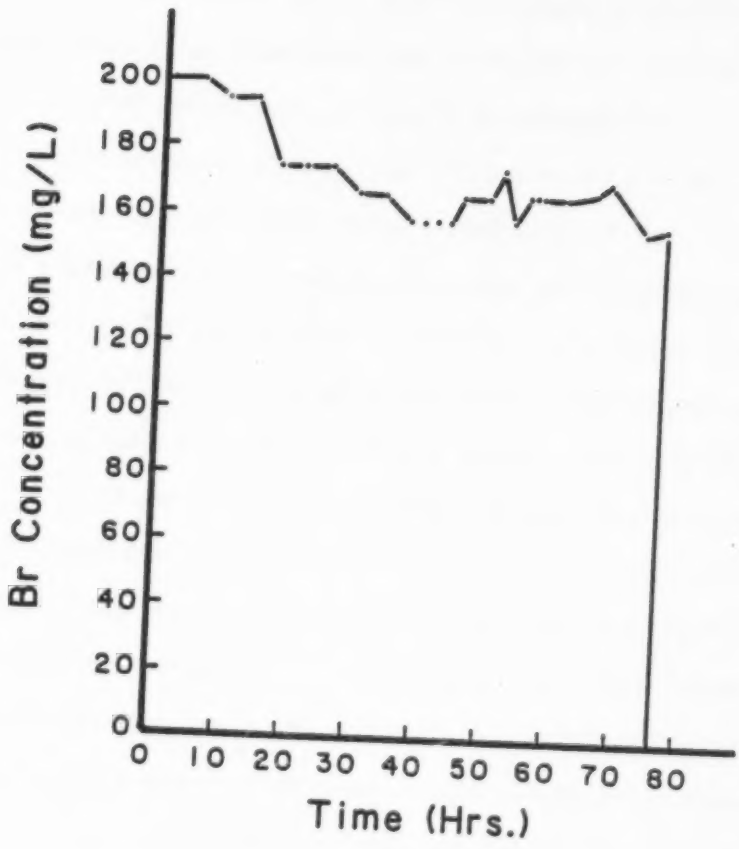

Figure 22. Injection well tracer concentration versus time during the first 80 hours of the two-well test.

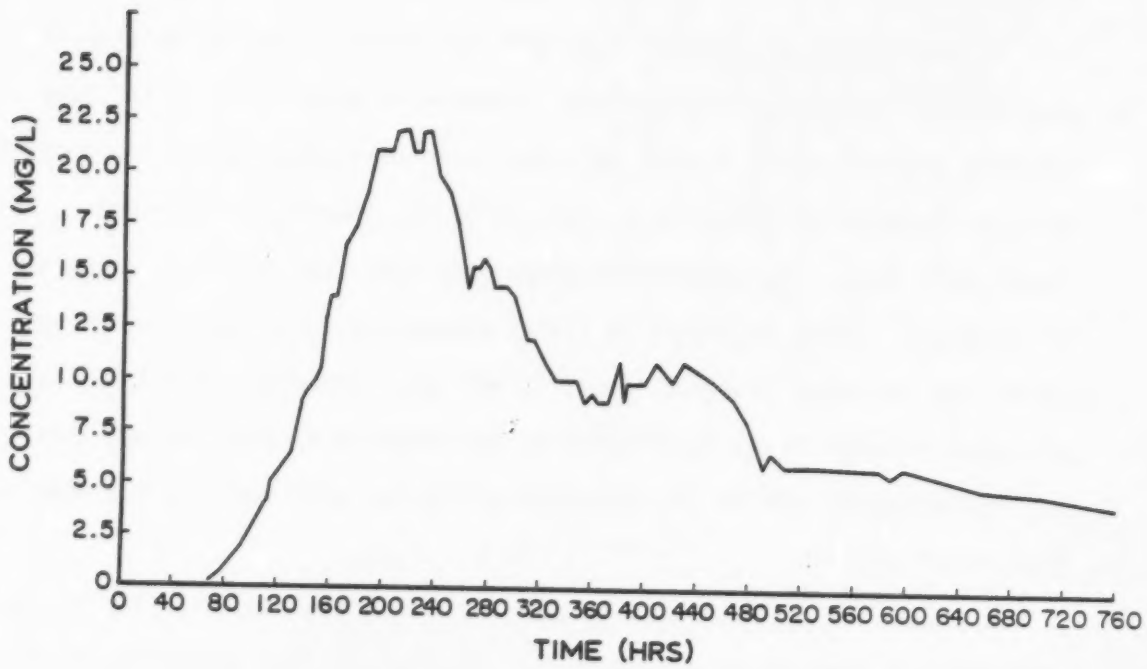

Figure 23. Measured tracer concentration versus time in the withdrawal well during the two-well test.

measurable tracer concentrations persisted throughout the 32.5 day experiment. The peak concentration occurred rather early in the experiment (~210 hours), and the curve had a well-defined "tail" that was still 15% of the peak value (~40 times the background value of 0.1 mg/l) when the experiment was terminated. Computer simulations (see below) indicated that the tailing was due to the late arrival of tracer being brought to the withdrawal well along the flow lines which follow the longer and larger arcs between the injection well and the withdrawal well shown in Figure 4.

Throughout the experiment, data were collected at the two multilevel observation wells shown in Figure 15. There were seven 0.9 m (3 ft) long isolated sampling zones in each well that were kept continuously mixed using peristaltic pumps on the surface, just as in the previously described single-well test. The peristaltic pumps were used also to obtain samples for analysis. Shown in Figure 24 (lines connecting dots) are breakthrough curves for the seven isolated levels in well E3. The data for well E5 is not shown because it was invalidated by the presence of drilling mud that was inadvertently left in the formation during the well construction process (Molz et al., 1985).

A tracer travel time analysis similar to that described for the single-well test and embodied in equations (6), (7), and (8) can be applied to the two-well test (Pickens and Grisak, 1981). When this is done, using the experimental data in Figure 24, the normalized hydraulic conductivity distribution shown in Figure 25 results. Although there are some differences, this distribution is quite similar to that shown in Figure 21 which resulted from the single-well test.

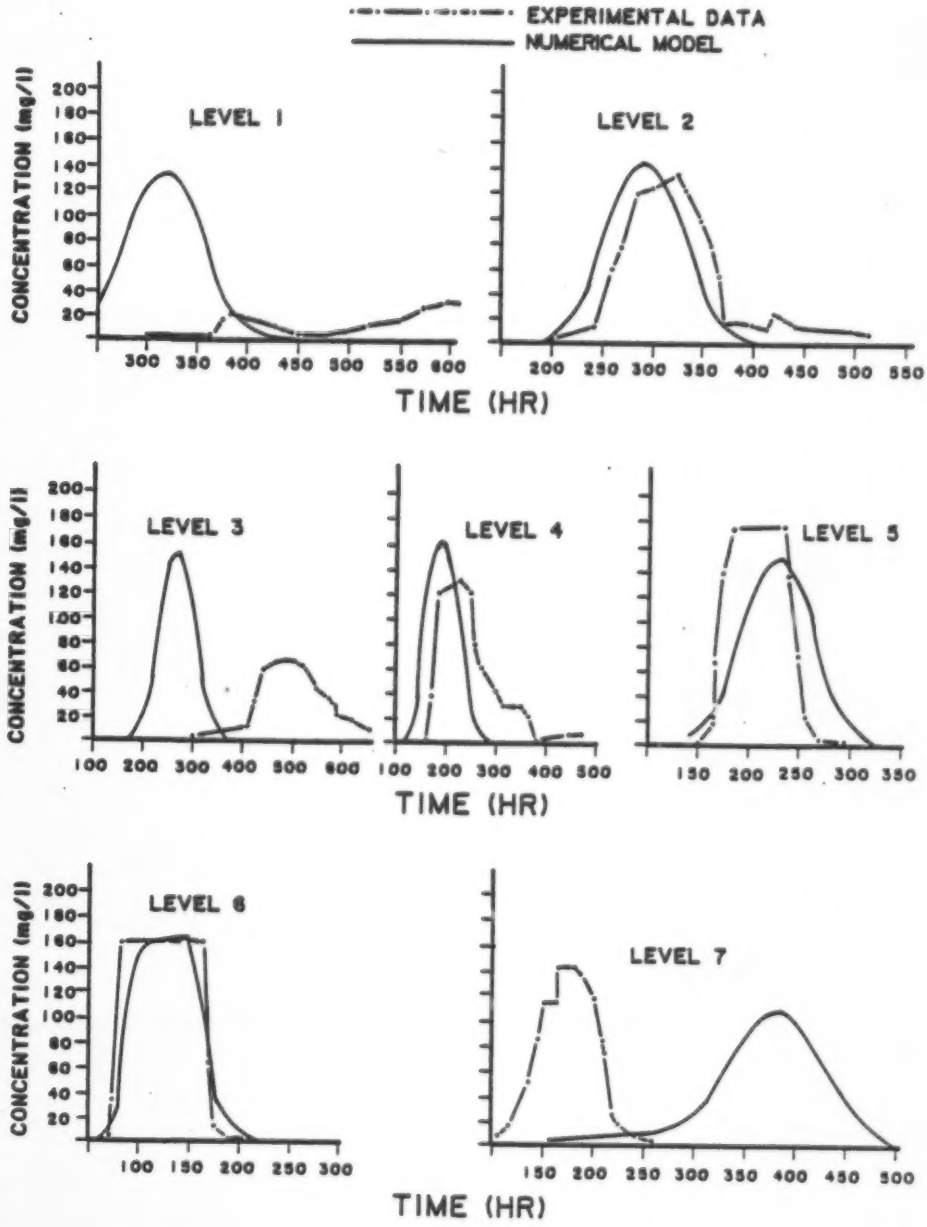

Figure 24. Measured (lines connecting dots) and predicted (full lines) breakthrough curves at the 7 levels of observation well E3.

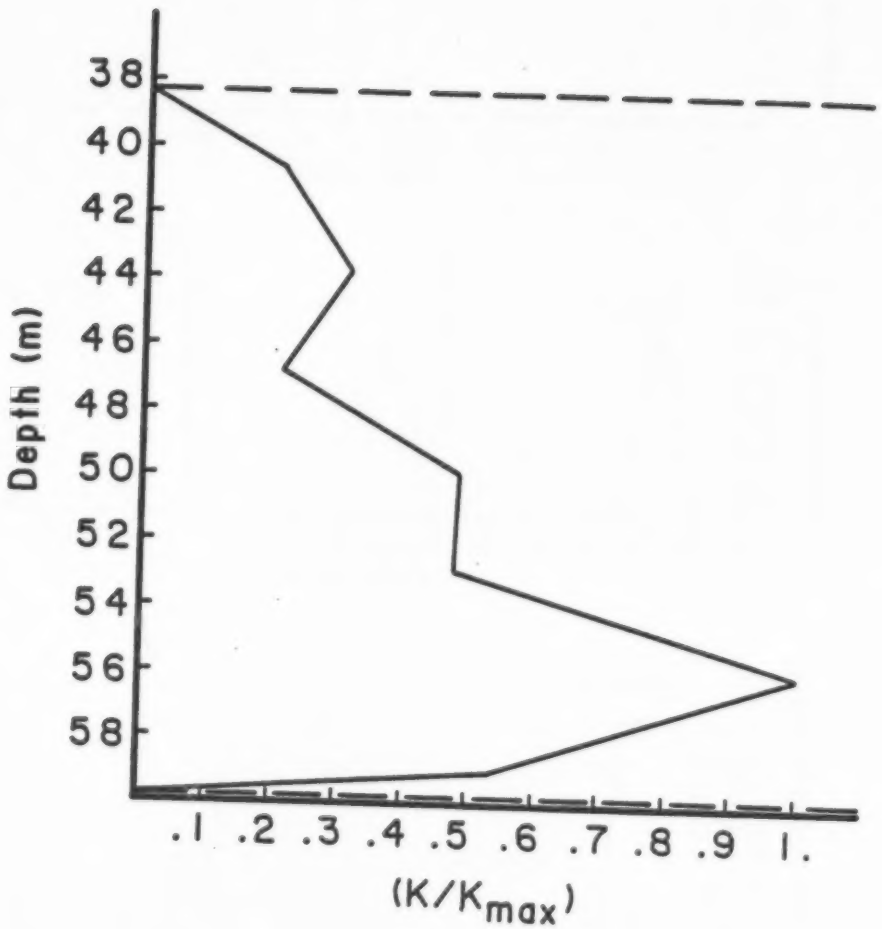

Figure 25. Normalized hydraulic conductivity distribution inferred from travel times measured during the two-well test.

Computer Simulation of Single-Well and Two-Well Test Results

The schematic diagram of tracer dispersion drawn in Figure 1 represents an advection-dominated process. One of the objectives of the research reported in this communication is to develop some indication of how much information concerning tracer dispersion is actually contained in normalized hydraulic conductivity distributions similar to the type determined in single-well and two-well tracer tests subject to the stratified aquifer approximation. Moreover, when such information is put into a mathematical model, how much of the dispersion process due to true hydrodynamic dispersion and other factors, such as spatial variations of hydraulic conductivity not allowed in the stratified aquifer assumption, is left unaccounted for? To begin to answer this question for aquifers where the required information is available, computer simulations for various experiments were developed which explicitly considered the vertical variation of horizontal hydraulic conductivity as determined by single-well or two-well tracer tests. Predictions of the computer models, which were made without "calibration" of any model parameters, were then compared with actual field results.

Simulation of Single-Well Tests

The first field tracer tests studied in this manner were the single-well tests performed by Pickens and Grisak (1981). This particular test was chosen for analysis because of the availability of very detailed data on hydraulic conductivity, local dispersivity and concentration distributions from the test. The computer model that was developed is called SWADM (Falta, 1984; Güven et al., 1985). It takes into account depth-dependent advection in the radial direction and local hydrodynamic dispersion in the

vertical and radial directions (Güven et al., 1985). The model is based on the equation given by

$$\frac{\partial C}{\partial t} + U_r \frac{\partial C}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left(r D_r \frac{\partial C}{\partial r} \right) + \frac{\partial}{\partial z} \left(D_z \frac{\partial C}{\partial z} \right) \qquad (9)$$

where r is the radial coordinate, $C = C(r,z,t)$ is the tracer concentration, $U_r = U_r(r,z)$ is the radial seepage velocity, $D_r = D_o + \alpha_r |U_R|$ is the radial dispersion coefficient, $D_v = D_o + \alpha_v |U_r|$ is the vertical dispersion coefficient, D_o is the effective molecular diffusion coefficient, and α_r and α_v are the radial and vertical local dispersivities.

The very detailed single-well tracer dispersion experiment of interest was performed in a shallow unconfined aquifer. A volume of 95.6 cubic meters of tracer-labeled water was injected into an 8.2 m thick aquifer at a rate of 3.2 m^3/hr for a period of 30 hours and then withdrawn at the same rate. Withdrawal began immediately at the end of injection. The previously-described samplers were located in the aquifer at observation stations 1, 2, 3, 4 and 6 m from the injection-withdrawal well. From the relative tracer arrival times at different elevations in the observation wells, a radial hydraulic conductivity distribution in the vertical (expressed as $K_i/\bar{K}$) was calculated. Additionally, Pickens and Grisak (1981) estimated the local longitudinal dispersivity at each sampling point and found the values to be fairly constant with an average magnitude of about 0.007 m. The $K/\bar{K}$ distribution inferred from the breakthrough data at the observation well at a distance of 1 m from the injection-withdrawal well in test SW1 was used in the SWADM simulation. This profile is shown in Figure 26. The actual unsteady injection concentration, shown in Figure 27, was used in the simulation (Pickens, 1983, personal communication), along with local radial and vertical dispersivities of 0.007 m. The value used for the

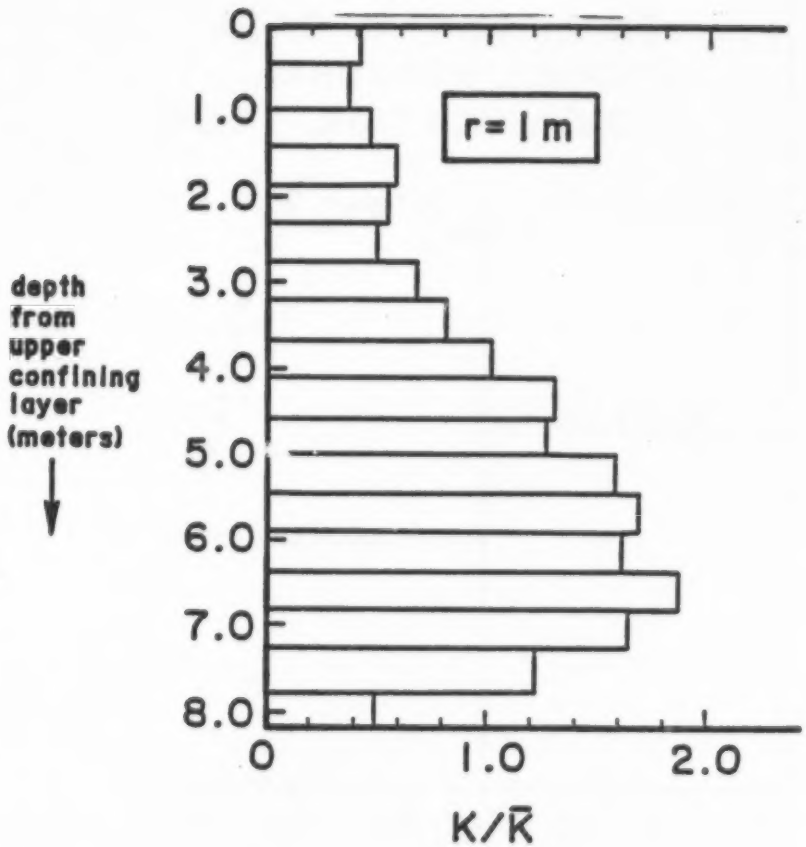

Figure 26. Hydraulic conductivity profile measured by Pickens and Grisak (1981) and used in the present calculations.

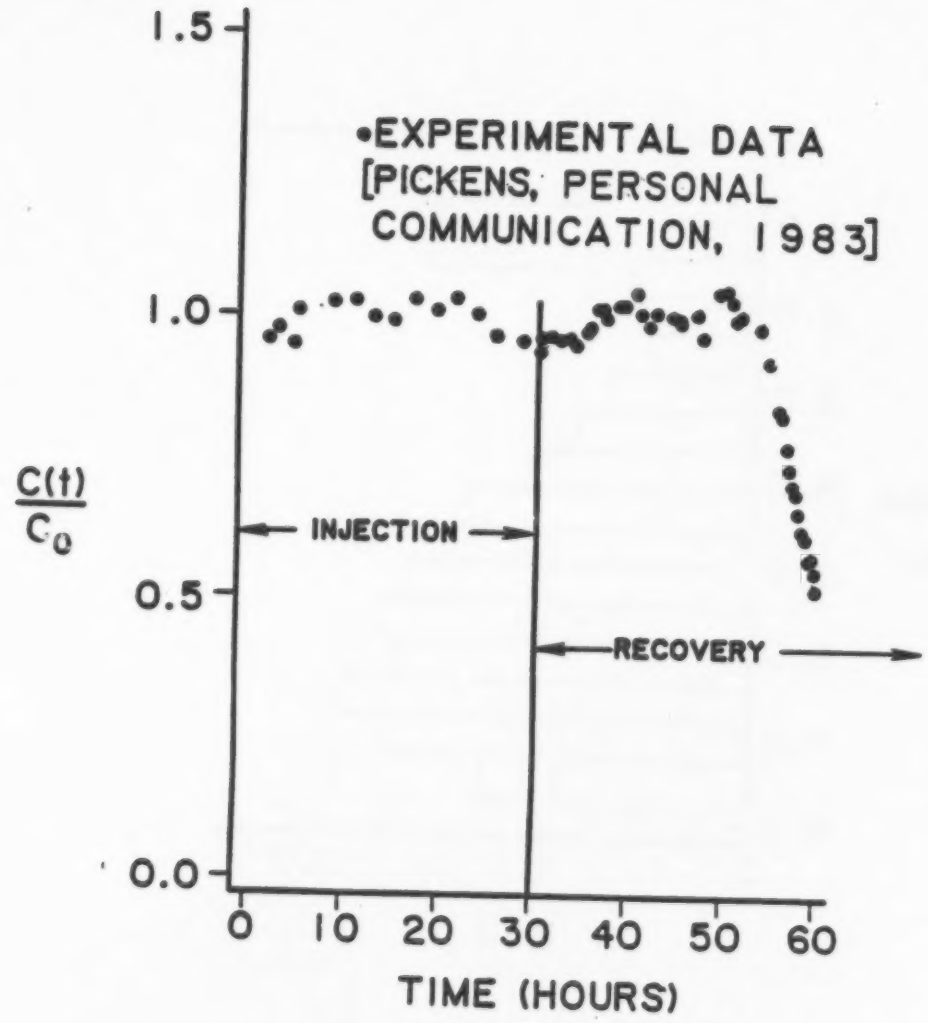

Figure 27. Unsteady injection concentration during the Pickens and Grisak (1981) single-well field experiment.

radial dispersivity is based on the observations, but the value used for the vertical dispersivity is arbitrary and it was chosen simply as a possible upper limit for this quantity in this case as discussed in more detail by Güven et al. (1985). The effects of the well radius and molecular diffusion were neglected. The porosity value used in the calculations was 0.38 as given by Pickens and Grisak (1981, page 1197).

In Figures 28 and 29, the actual flow-weighted breakthrough curves from observation wells located 1 and 2 m from the injection-withdrawal well respectively (Pickens and Grisak, 1981b) are shown along with the flow-weighted breakthrough curves calculated by SWADM. (The flow-weighted concentration, $\hat{C}$ is defined as $\hat{C} = \int_0^B (K(z)/\bar{K})Cdz/B$, where B is the aquifer thickness.) In Figure 29, the wavy appearance of the computed curve for a time greater than about 10 hours is due to the unsteady injection concentration used in the simulation. The experimental concentration versus time data measured at the injection-withdrawal well is shown in Figure 30 along with the results of the SWADM simulation using the unsteady input concentrations. The early part of the experimental data seems to show a large amount of scatter; however, this part of the curve is closely modeled by SWADM using the actual unsteady injection concentration. The later part of the breakthrough curve is underestimated by SWADM. The reasons for this are not clear. One possible contributing factor could be the presence of small-scale, three-dimensional, very-low-permeability lenses embedded in the aquifer, which the present model does not take into account. These lenses could act as temporary storage zones for the tracer which may diffuse into these zones during injection and then move out slowly during withdrawal, leading to larger concentrations during withdrawal than predicted by SWADM. Another possible contributing factor for the behavior noted above is that

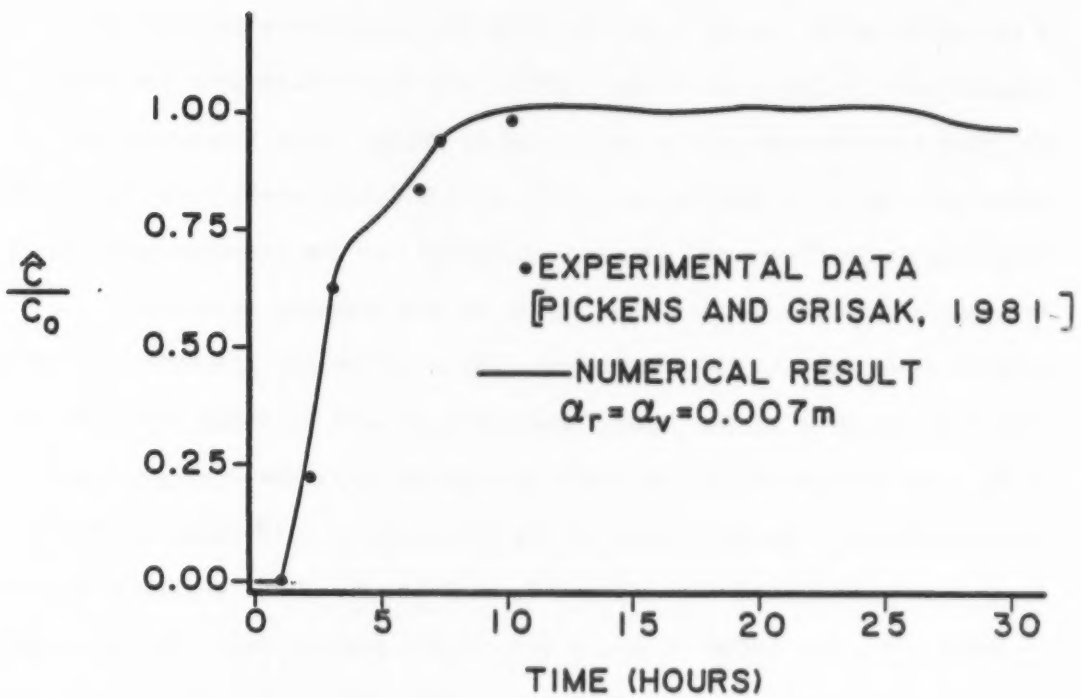

Figure 28. Comparison of SWADM results with field data for the flow-weighted concentration from an observation well one meter from the injection-withdrawal well.

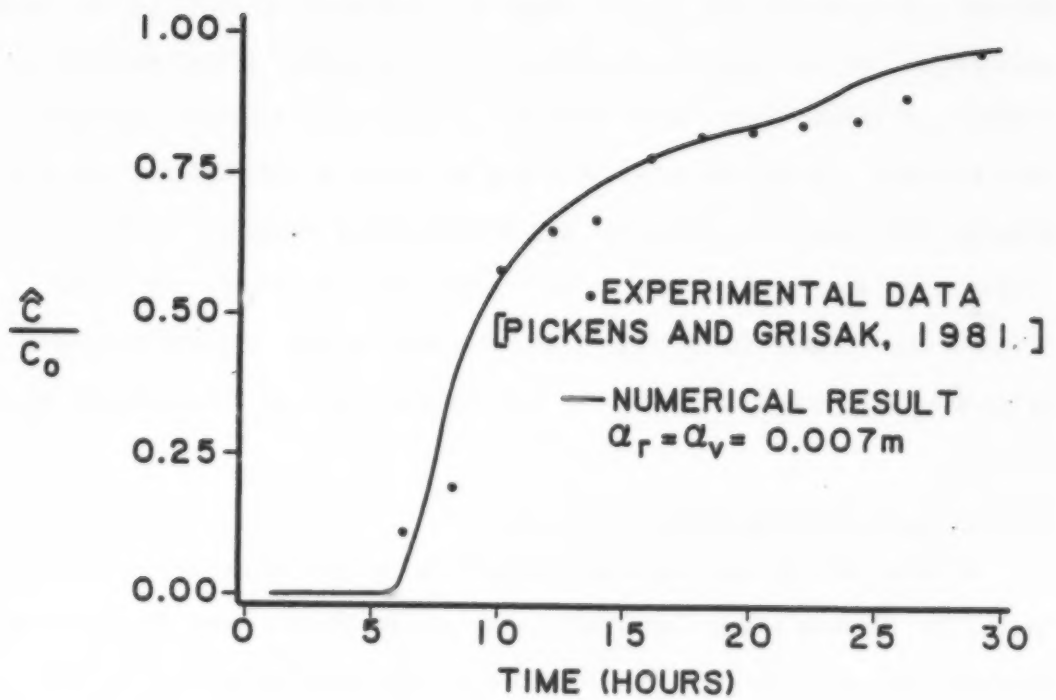

Figure 29. Comparison of SWADM results with field data for the flow-weighted concentration from an observation well two meters from the injection-withdrawal well.

according to the measured data, approximately 2.5 percent more tracer was shown to have been withdrawn than was injected. While this is certainly not a large experimental error for a field experiment (in fact it is quite small), it is enough to have significantly changed the slope of the later part of the curve if that is where the error occurred. Since a mass balance was not satisfied perfectly during this experiment, the net area under the experimental curve is greater than the area under the calculated curve. However, in obtaining the results shown in Figures 28, 29, and 30, no "model calibration" of any type was performed. Only parameter values measured by Pickens and Grisak (1981) were utilized. The resulting curves represent very accurate simulations which indicate an advection-dominated dispersion process with local dispersivities approaching those measured in the laboratory. As also discussed in more detail by Molz et al. (1983) and Güven et al. (1984), it is clear that if a full-aquifer dispersivity were calculated from these data it would not represent a physical property of the aquifer.

Simulation of Two-Well Tests

To date, simulations have been performed for two separate two-well tests, the Pickens and Grisak (1981) test and the Mobile test described in a previous section. Only the Mobile two-well test simulation will be presented in detail because the conclusions are similar to those that result from simulation of the Pickens and Grisak (1981) test but are somewhat more significant because of the larger scale of the experiment.

In our simulation of the E1-I2 two-well test we chose to employ the single-well test as a means for inferring the hydraulic conductivity distribution in a relatively small aquifer region between the injection well and a multilevel observation well. The two-well experiment was then used to

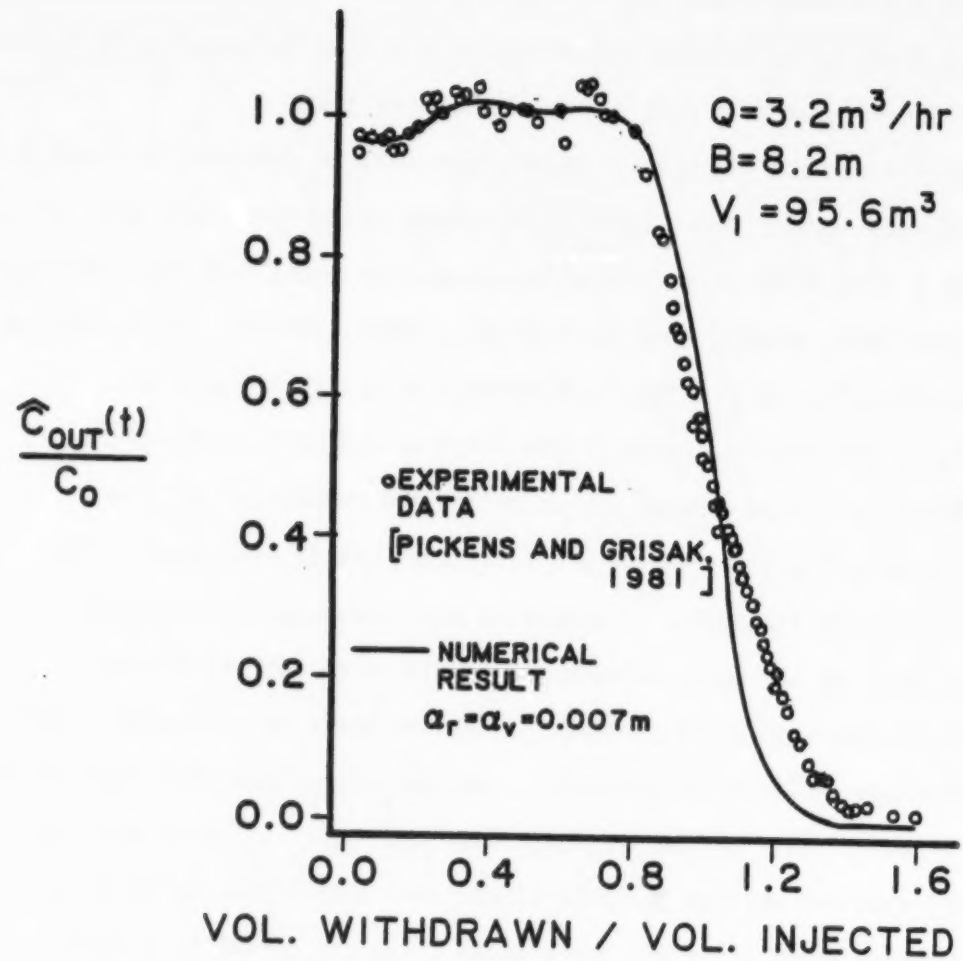

Figure 30. Comparison of SWADM results with field data for the concentration leaving the injection-withdrawal well.

test the prediction capability over a relatively large aquifer region, based on the vertical distribution of hydraulic conductivity inferred from the single-well test shown in Figure 21. This procedure helps to define what is actually being measured during a single-well test and over what travel distances such a measurement might retain some meaning. It also provides insight concerning fundamental properties of the flow fields which were established at the Mobile site during the various tests.

Two separate and independent models were used to simulate the results of the two-well test. Under contract to Auburn University, GeoTrans, Inc., developed a three-dimensional advection-dispersion model that took advantage of our particular geometry (Huyakorn et al., 1986a, 1986b). The aquifer was divided vertically into 12 layers of varying thicknesses (Table 3), depending on the rate of change of the relative hydraulic conductivity distribution, and flow between the injection and production wells was assumed to be stratified, steady and horizontal within each layer. The advection pattern for such a situation is well known (Davis and DeWiest, 1966, p. 209), so the Darcy velocity, U, could be calculated at any particular point within the 12-layer system (Huyakorn et al., 1986a, 1986b). Given the known velocity distribution, the advection-dispersion equation was solved using a finite element approach (Huyakorn et al., 1986b) with the governing equation written in three-dimensional curvilinear coordinates (s,n,z), where s and n are the coordinates along and normal to a local streamline, and z is the vertical coordinate. In this system the transformed advection-dispersion equation is given by

$$\frac{1}{h_2}\frac{\partial}{\partial s}\left(h_2 D_s \frac{\partial C}{\partial s}\right) + \frac{1}{h_1}\frac{\partial}{\partial n}\left(h_1 D_n \frac{\partial C}{\partial n}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C}{\partial z}\right) - \frac{U}{\theta}\frac{\partial C}{\partial s} - \frac{\partial C}{\partial t} = 0 \qquad (10)$$

Table 3. Two-well test parameters supplied to GeoTrans, Inc. for their 3-dimensional simulations based on the advection-dispersion equation.

(Normalized Hydraulic Conductivity Distribution)

Layer # (i)	Layer Center (z_i)	Layer Thickness	Normalized Cond. ($K(z_i)/K_{max}$)
12	20.4 m	2.40 m	0.15
11	17.97	2.46	0.31
10	15.62	2.24	0.34
9	13.37	2.25	0.38
8	11.50	1.50	0.48
7	10.00	1.50	0.57
6	8.50	1.50	0.51
5	7.00	1.50	0.44
4	5.50	1.50	0.72
3	4.00	1.50	1.00
2	2.50	1.50	0.65
1	0.87	1.75	0.25

(Additional Parameters)

Longitudinal dispersivity	0.15 m
Transverse (horizontal) dispersivity	0.05 m
Transverse (vertical) dispersivity	0.01 m
Tracer injection time	3.19 days
Total injection time	32.5 days
One-half well spacing	19.14 m
Radius of injection and production wells	0.08 m
Injection and production rates	0.9464 m^3/min
Porosity	0.35
Aquifer thickness	21.6 m
Molecular diffusion coefficient	$1x10^{-9}$ m^2/s
Screen location (Injection well)	Fully penetrating
Screen location (Withdrawal well)	Fully penetrating
E3 observation well coordinates	(x=13.56 m, y = 0)

where D_s, D_n and D_z are principal components of the hydrodynamic dispersion tensor in the longitudinal, transverse and vertical directions, respectively, and h_1 and h_2 are the scale factors of the curvilinear coordinate system (Huyakorn et al., 1986a). The dispersion coefficients are defined as

$$D_s = \alpha_L \, U/\theta + D_o \tag{11a}$$

$$D_n = \alpha_T \, U/\theta \tag{11b}$$

$$D_z = \alpha_z \, U/\theta + D_o \tag{11c}$$

where α_z is the vertical dispersivity, and U is a function of s, n and z. Solution of equation (10) enables one to predict the tracer concentration in the production well as a function of time and also the tracer concentrations as functions of time at each level in the multilevel observation well E3. The actual information supplied to GeoTrans is listed in Table 3. The Cartesian coordinates listed are based on Figure 4.

The second model used to simulate the two-well test is called the two-well advection model (TWAM) and was developed at Auburn University (Falta, 1984; Güven et al., 1986). A Lagrangian solution method is used in this model based on the travel times of tracer along various flow lines from one well to the other. In this model, it is assumed that the aquifer is horizontal, confined, of constant thickness and porosity, and perfectly stratified in the vicinity of the test wells. TWAM takes into account the depth-dependent advection in the horizontal planes, but neglects completely any local hydrodynamic dispersion. Thus any simulations resulting from application of TWAM will yield dispersed concentration distributions based solely on differential advection, which is also called shear flow (Fischer et al., 1979).

Shown in Figure 31 are the results of the 3-dimensional dispersion simulation and the advection simulation using the model called TWAM (Güven et al., 1986). Both models do a remarkably good job of predicting the

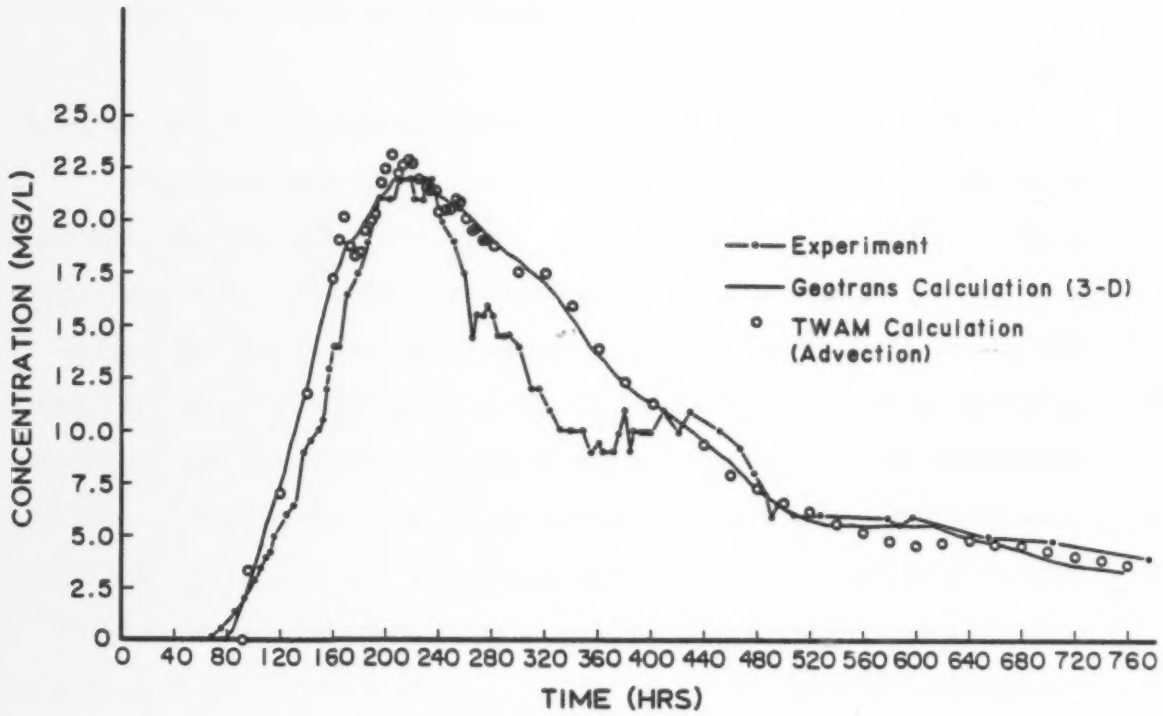

Figure 31. Results of various simulations of the two-well test. No "calibration" or curve-fitting of any type was used.

recovery concentrations during the two-well test. Since the two independent predictions agreed quite well, one can conclude that local hydrodynamic dispersion played a very minor role in determining the time distribution of tracer concentration in the withdrawal well. The entire experiment, which involved estimated travel distances over individual flow paths ranging from 38.3 m to about 90 m in the most permeable layer, was highly advection-dominated. The dominant role of advection in the two-well test was also noted earlier by Hoopes and Harleman (1967) for the case of a homogeneous aquifer.

We would like to emphasize that no prior calibration was done in order to arrive at the results shown in Figure 31. All of the information supplied to our subcontractor is listed in Table 3. They did not know the result of the experiment they were attempting to simulate. With the exception of the dispersivity values and the porosity, all of the information contained in Table 3 was measured directly in the field or calculated from field measurements. The dispersivity values were chosen arbitrarily to have relatively small finite values because the 3-D model would develop numerical dispersion and/or excessive CPU time problems if the dispersivity got too close to zero. Porosity was measured in the laboratory on disturbed core samples obtained from well E3 during drilling operations. The seven samples were compacted lightly and the porosity measured based on the determination of solids specific gravity and saturated water content. The average for well E3 was 0.41. It was reasoned that this value would likely be higher than the undisturbed in-situ values, so an effective porosity of 0.35 was chosen prior to any simulations. The 3-D model result in Figure 31, based on the 0.35 porosity value, was obtained from a single computer run which

required 8.5 hours of CPU time on a Prime 550-2 minicomputer (Huyakorn et al., 1986b). Runs at Auburn University based on identical data using TWAM (Falta, 1984; Güven et al., 1986) were performed independently of the GeoTrans run.

The calculated withdrawal concentration functions in Figure 31 were obtained from a flow-weighted average of the concentrations along the withdrawal well screen and thus is a vertically integrated quantity. A comparison between concentration breakthrough curves measured at the 7 discrete levels of observation well E3 and those predicted by the 3-D model are shown in Figure 24. At levels 2, 4, 5, and 6, the agreement is good, while at levels 3 and 7 it is poor. A valid comparison cannot be made at level 1 because of an apparent leak in the tubing used to obtain the level 1 samples (Molz et al., 1985). The mixed results of Figure 24 are not unexpected because one would not expect the normalized hydraulic conductivity distribution shown in Figure 21 to remain completely invariant in a fluvial aquifer over the 38.3 m separation between the injection and production wells. However, it is significant that the integrated prediction (Figure 31) remains quite good.

The prediction of concentration versus time in the withdrawal well is sensitive to the normalized hydraulic conductivity distribution. Shown in Figure 32 is the withdrawal concentration breakthrough that would result if one assumed a homogeneous aquifer with a normalized hydraulic conductivity of unity throughout. In such a situation, one would observe a longer travel time for the first arrival of the tracer at the withdrawal well and a much higher peak concentration than was realized during the actual experiment. However, the general behavior of the tail of the curve does not appear sensitive to the details of the normalized hydraulic conductivity distribution.

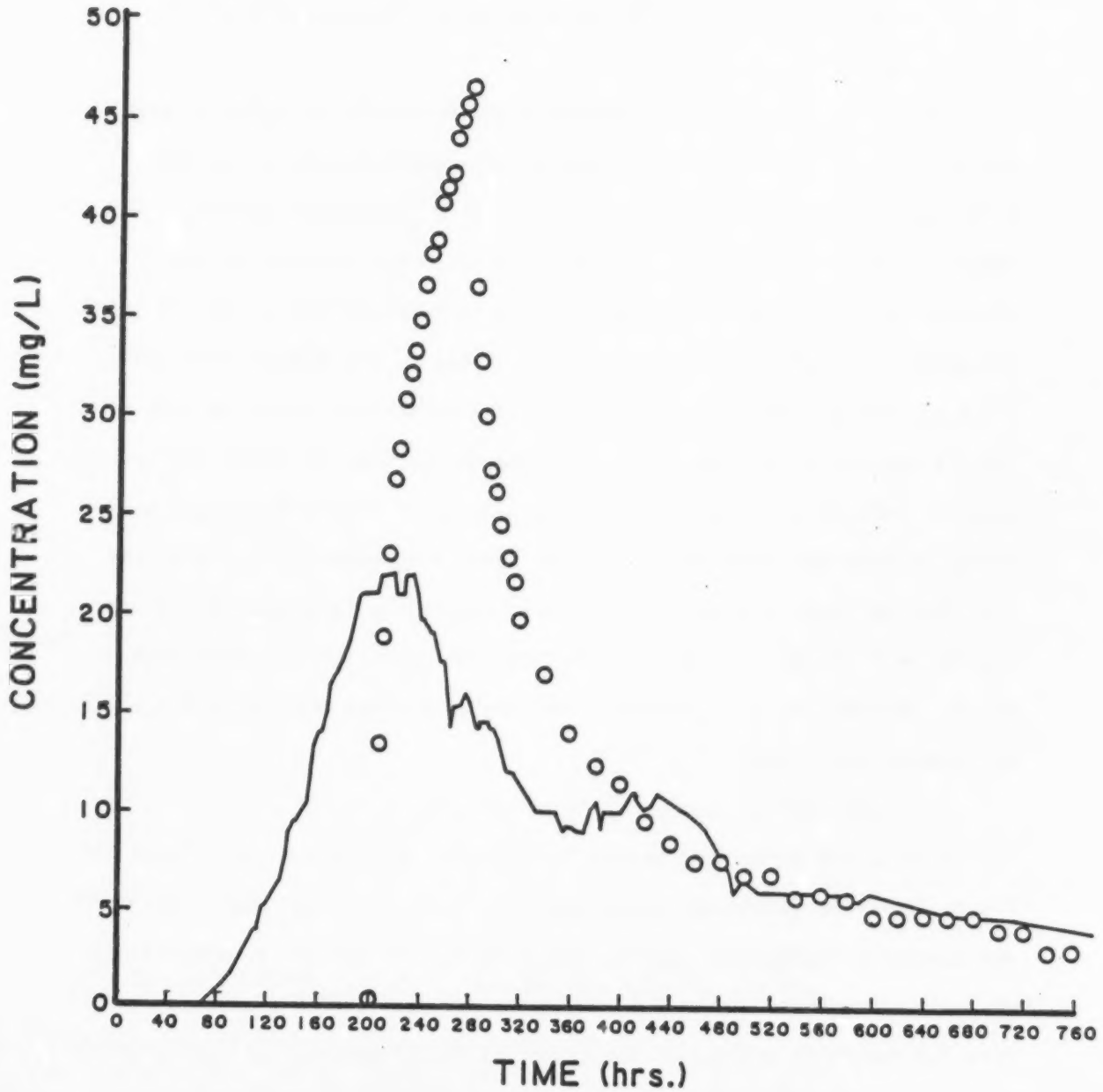

Figure 32. Calculated tracer concentration versus time in the withdrawal well based on an assumed homogeneous, isotropic aquifer with no local dispersion (circles) shown together with the results of the present two-well test (full line).

A good fit to the data results if one assumes a full-aquifer longitudinal dispersivity of 4 m (Huyakorn et al., 1986b).

Further understanding of the implications of the data and computations contained in Figures 24 and 31 can be obtained by selecting a normalized hydraulic conductivity distribution so that the computed and measured breakthrough curves of Figure 24 are made to agree with each other as far as peak arrival times are concerned. (Essentially, this is equivalent to using the two-well test itself to estimate the normalized hydraulic conductivity distribution.) This was discussed previously, and the distribution shown in Figure 25 was obtained. There is not a tremendous difference between the normalized hydraulic conductivity distributions shown in Figures 21 and 25, but the Figure 25 conductivity values in the upper half of the aquifer are smaller. A TWAM simulation of the withdrawal well concentrations based on the Figure 25 distribution is shown in Figure 33. While the rising limb of the breakthrough curve is not simulated as well, there is closer agreement between the data and computations for the falling limb than was obtained previously (Figure 31) using the normalized hydraulic conductivity distribution shown in Figure 21. Overall, the simulations shown in Figures 31 and 33 are of comparable quality.

The single-well and two-well test simulations discussed in this section pertained to different aquifers in widely separated locations. The single-well test was performed in a clean, sandy, glaciofluvial aquifer in Canada, while the two-well test was performed in a fluvial, low-terrace deposit containing sand with appreciable amounts of clay. Both simulations were quite accurate in an integrated sense and consistent with an advection-dominated (shear flow) dispersion process. When advection was considered

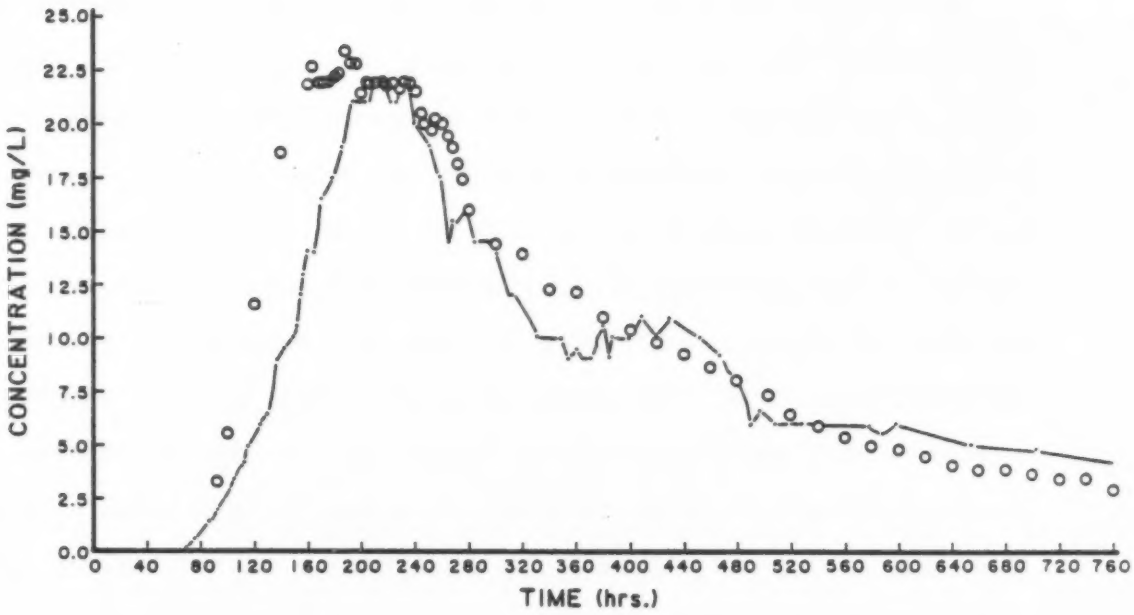

Figure 33. Comparison of measured and calculated tracer concentration versus time in the withdrawal well based on the normalized hydraulic conductivity distribution shown in Figure 25.

explicitly, large, scale-dependent, full-aquifer dispersivities were not required.

Discussion and Conclusions

In the recent past, some hydrologists advocated the use of single-well or two-well tracer dispersion tests as a means for measuring full-aquifer longitudinal dispersivity. However, our analyses of single- and two-well tests in stratified aquifers indicate that if this is done, the resulting number will have little physical meaning. In the case of single-well tests, the full-aquifer breakthrough curves measured in observation wells are determined mainly by the hydraulic conductivity profile in the region between the injection-withdrawal well and an observation well if the travel distance between the injection-withdrawal well and the observation well is typical of most test geometries. Thus, information about the conductivity profile is necessary for meaningful test interpretation. The relative concentration versus time data recorded at the injection-withdrawal well itself is primarily a measure of the combined local and (perhaps?) semi-local dispersion which has taken place during the experiment. Of course, the effects of such dispersion will depend in part on the hydraulic conductivity distribution in the aquifer, and in part on the size of the experiment. As the size of the experiment increases, the effects of local vertical dispersion will become larger compared to the effects of local radial dispersion (Güven et al., 1985).

The two-well test simulations show that the concentration versus time breakthrough curve measured at the withdrawal well would be very sensitive to variations of the hydraulic conductivity in the vertical. Without the use of multilevel observation wells, the test would give little useful information about the hydraulic or dispersive characteristics of the

aquifer, such as aquifer stratification or values of local dispersivities. Factors such as the length of the injection period, the use of recirculation, and the physical size of the experiment all have a strong effect on the breakthrough curve measured at the withdrawal well, making the interpretation of field results difficult, unless aquifer stratification is measured and properly taken into account (Güven et al., 1986).

Based on the above observations and the large values for full-aquifer dispersivities that consistently result from calibrated areal groundwater transport models, we believe that the following working conclusions are warranted.

I. Local longitudinal hydrodynamic dispersion plays a relatively unimportant role in the transport of contaminants in aquifers. Differential advection (shear flow) in the horizontal direction is much more important.

II. The concept of full-aquifer dispersivity used in vertically-averaged (areal) models will not be applicable over distances of interest in most contamination problems. If one has no choice but to apply a full-aquifer dispersion concept, the resulting dispersivity will not represent a physical property of the aquifer. Instead, it will be an ill-defined quantity that will depend on the size and type of experiment used for its supposed measurement.

III. Because of conclusion II, it makes no sense to perform tracer tests aimed at measuring full-aquifer dispersivity. If an areal model is used, the modeler will end up adjusting the dispersivity during the calibration process anyway, independent of the measured value.

IV. When tracer tests are performed, they should be aimed at determining the hydraulic conductivity distribution. Both our theoretical and experimental work have indicated that the variation of horizontal hydraulic conductivity with respect to vertical position is a key aquifer property related to spreading of contaminants.

V. Two- and three-dimensional modeling approaches should be utilized which emphasize variable advection rates in the horizontal direction and hydrodynamic dispersion in the transverse directions along with sorption and microbial/chemical degradation.

VI. In order to handle the more advection-dominated flow systems described in conclusion V, one will have to utilize or develop numerical algorithms that are more resistant to numerical dispersion than those utilized in the standard dispersion-dominated models.

As discussed in the introduction, much of our contemporary modeling technology related to contaminant transport may be viewed as an attempt to apply vertically homogeneous aquifer concepts to real aquifers. Real aquifers are not homogeneous, but they are not perfectly stratified either. What we are suggesting, therefore, is that the time may have arrived to begin changing from a homogeneous to a vertically-stratified concept when dealing with contaminant transport, realizing fully that such an approach will be interim in nature and not totally correct. However, our performance and simulation of several single- and double-well tracer tests suggests that the stratified approach is much more compatible with valid physical concepts, and at least in some cases, results in a mathematical model that has a degree of true predictive ability. Nevertheless, real-world applications will undoubtedly require calibration, which in the stratified approach would

involve varying the hydraulic conductivity distribution rather than the longitudinal dispersivity. The benefit is that when calibrating the K distribution, one is dealing with the physical property that probably dominates the dispersion process.

The change from a vertically-homogeneous to a vertically-stratified approach will not be easy from a field measurement viewpoint nor will it be inexpensive. The work of Pickens and Grisak (1981) and the work described herein has developed some prototype technology and methodology for obtaining the type of information shown in Figure 34. This figure presents the results of a preliminary analysis of all single-well tests to date that have been performed at the Mobile site and analyzed in the vertical plane shown in Figures 15 and 34. The mean locations in the aquifer where the tests took place are indicated in the bottom half of the figure.

Examination of the K/K_{max} plots in Figure 34 reveal some interesting trends. A high hydraulic conductivity zone in the bottom third of the aquifer is evident in all four of the tests. A similar high hydraulic conductivity zone appeared in the top third of the aquifer during the E5-E1 test and the E10-E9 test, but not in the two tests conducted in the vicinity of I2. If one attempted to "fit" a stratified mathematical model to the situation illustrated in Figure 34, the strict definition of a stratified aquifer could not be maintained. As a practical necessity, one would have to postulate a "local" or "quasistratified concept" wherein flow was generally horizontal on the average with the vertical distribution of horizontal hydraulic conductivity gradually shifting from one distribution to the other. There are, however, other considerations that may make the "approximately stratified" idealization work better than expected. While the imposed flow was observed to be locally stratified in the present

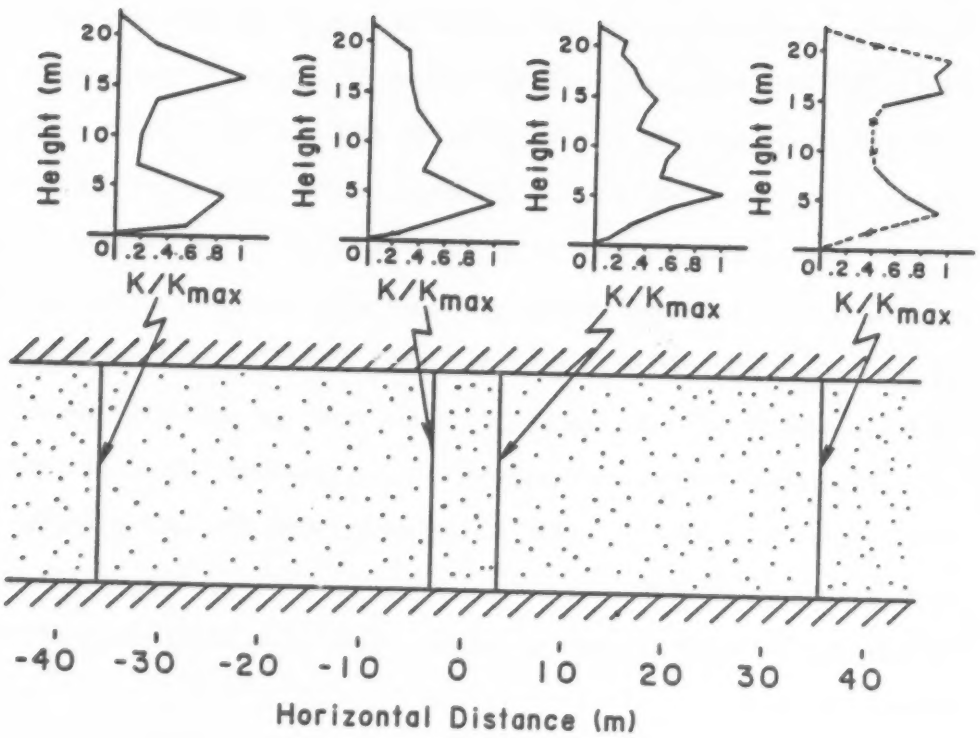

Figure 34. Preliminary results of four single well tests performed at the Mobile site. All stations shown are situated at approximately the same vertical plane.

experiments and in the experiments of Pickens and Grisak (1981), this does not necessarily mean that the aquifer hydraulic conductivity distribution is also stratified around the localities where the tests were performed; areal variations of hydraulic conductivity could still be present at each level of the aquifer around a test well. However, an overall stratified flow pattern could still develop in a confined aquifer even if the hydraulic conductivity distribution is not perfectly stratified. This is because the flow is forced to be horizontal on the average in a confined aquifer, and a quasi-stratified flow may develop along various flow paths in response to the effective average value of the hydraulic conductivity at each level of the aquifer along the flow path, as observed in the field experiments discussed above. This behavior seems to be supported also by the results of some ongoing numerical solute transport experiments presently being performed at Auburn University. In a three-dimensional numerical experiment in a confined aquifer with a completely random computer-generated synthetic hydraulic conductivity distribution, it was observed, somewhat surprisingly, that a quasistratified flow field developed along the entire travel path of a contaminant slug introduced numerically into the aquifer, which resulted in considerable longitudinal spreading (shear flow dispersion) of the contaminant plume.

A question that should be considered further relates to the practical feasibility of performing the tracer tests required by the stratified approach. In most situations we view tracer tests as feasible technically but only marginally feasible in a routine practical sense. As discussed in the section on multilevel sampling wells, the unavailability of widely accepted commercial equipment is a major practical impediment. However, that problem may disappear in the near future, and the need to consider

vertical aquifer property variations is very real. As illustrated by the field work of Osiensky, Winter and Williams (1984), the use of full-aquifer dispersion concepts to model what is essentially a shear flow dispersion process does not result in a conservative estimate of contaminant concentrations. Instead, the model induces a large amount of artificial mixing which often leads to an unrealistically-rapid dilution of a contaminant plume. Such an analysis at a site in central Wyoming concluded that the 1000 mg/l sulfate contour line was located at a maximum distance of about 450 m downgradient from the source. However, further study by Osiensky et al. (1984) which considered the structure of the fluvial aquifer in more detail showed that there were portions of the aquifer 1020 m downgradient that contained sulfate concentrations in excess of 5000 mg/l. Occurrence of this kind of potential mistake can be minimized only by including more information about the actual geometry and hydraulic conductivity distribution regardless of whether a mathematical model is part of the analysis. The interim stratified aquifer approach to tracer test analysis and modeling discussed herein is meant to be a step in that direction.

One obvious implication of our study is that any type of groundwater contamination analysis and reclamation plan will be difficult, expensive and probably unable to meet all of the desired objectives in a reasonable time frame. This reinforces the time-honored saying that 0.0283 kg (1 oz) of prevention is worth 0.454 kg (1 lb) of cure, which in the case of groundwater pollution is probably an understatement. One can not over-emphasize the advantages of preventing such pollution whenever it is feasible.

References

Alpay, O. A. 1972. A practical approach to defining reservoir heterogeneity. J. Petrol. Technol. v. 20, pp. 841-848.

Anderson, M. P. 1983. Movement of contaminants in groundwater, groundwater transport: advection and dispersion. In Groundwater Contamination: Product of a Technological Society, Natl. Res. Counc. Geophys. Study, pp. 37-45. National Academy Press. Washington, D.C.

Buscheck, T. A., C. Doughty, and C. F. Tsang. 1983. Prediction and analysis of a field experiment on a multilayered aquifer thermal energy storage system with strong buoyancy flow. Water Resour. Res. v. 19, pp. 1307-1315.

Dagan, G. 1984. Solute transport in heterogeneous porous formations. Journal of Fluid Mechanics v. 145, pp. 151-177.

Davis, S. N., and R. J. M. DeWiest. 1966. Hydrogeology. John Wiley and Sons, New York. 463 pp.

Falta, R. W. 1984. Analysis and Interpretation of Single-Well and Two-Well Tracer Dispersion Experiments in Stratified Aquifers. M.S. Thesis. Department of Civil Engineering, Auburn University, Alabama. 101 pp.

Fischer, H. B., E. J. List, R. C. Y. Koh, J. Imberger, and N. H. Brooks. 1979. Mixing in Inland and Coastal Waters. Academic Press, New York. 483 pp.

Freeze, R. A., and J. A. Cherry. 1979. Groundwater. Prentice-Hall. 604 pp.

Fried, J. J. 1975. Groundwater Pollution. Elsevier, New York. 330 pp.

Gelhar, L. W., A. L. Gutjahr, and R. L. Naff. 1979. Stochastic analysis of macrodispersion in a stratified aquifer. Water Resour. Res. v. 15, pp. 1387-1397.

Gelhar, L. W., and C. L. Axness. 1983. Three-dimensional stochastic analysis of macrodispersion in aquifers. Water Resour. Res. v. 19, pp. 161-180.

Güven, O., F. J. Molz, and J. G. Melville. 1984. An analysis of dispersion in a stratified aquifer. Water Resour. Res. v. 20, pp. 1337-1354.

Güven, O., R. W. Falta, F. J. Molz, and J. G. Melville. 1985. Analysis and interpretation of single-well tracer tests in stratified aquifers. Water Resour. Res. v. 21, pp. 676-684.

Güven, O., R. W. Falta, F. J. Molz, and J. G. Melville. 1986. A simplified analysis of two-well tracer tests in stratified aquifers. Ground Water v. 24, pp. 64-82.

Güven, O. 1986. Conditional simulations of solute transport in a stratified aquifer. EOS v. 67, p. 283.

Hoeksema, R. J., and P. K. Kitanidis. 1984. An application of the geostatistical approach to the inverse problem in two-dimensional groundwater modeling. Water Resour. Res. v. 20, pp. 1003-1020.

Hoopes, J. A., and D. R. Harleman. 1967. Wastewater recharge and dispersion in porous media. J. Hyd. Div., ASCE v. 93, pp. 51-71.

Huyakorn, P. S., P. F. Andersen, O. Güven, and F. J. Molz, 1986a. A curvilinear finite element model for simulating two-well tracer tests and transport in stratified aquifers. Water Resour. Res. v. 22, in press.

Huyakorn, P S., P. F. Andersen, F. J. Molz, O. Güven, and J. G. Melville. 1986b. Simulations of two-well tracer tests in stratified aquifers at the Chalk River and the Mobile sites. Water Resour. Res. v. 22, in press.

Journel, A. G., and C. T. Huijbregts. 1978. Mining Geostatistics. Academic Press, New York.

Kitanidis, P. K., and E. G. Vomvoris. 1983. A geostatistical approach to the inverse problem in groundwater modeling (steady state) and one-dimensional simulations. Water Resour. Res. v. 19, pp. 677-690.

Konikow, L. F. 1986. Predictive accuracy of a ground-water model. Ground Water v. 24, pp. 173-184.

Matheron, G., and G. deMarsily. 1980. Is transport in porous media always diffusive? A counterexample. Water Resour. Res. v. 16, pp. 901-917.

Moltyaner, G. L., and R. W. D. Killey. 1986. Scale independence of dispersivity and a dry-access-tube monitoring technique. Water Resour. Res. v. 22, in press.

Molz, F. J., J. G. Melville, O. Güven, and A. D. Parr. 1983. Aquifer thermal energy storage, an attempt to counter free thermal convection. Water Resour. Res. v. 19, pp. 922-930.

Molz, F. J., J. G. Melville, O. Güven, R. D. Crocker, and K. T. Matteson. 1985. Design and performance of single-well tracer tests at the Mobile site. Water Resour. Res. v. 21, pp. 1497-1502.

Molz, F. J., O. Güven, and J. G. Melville. 1983. An examination of scale-dependent dispersion coefficients. Ground Water v. 21, pp. 715-725.

Molz, F. J., O. Güven, J. G. Melville, R. D. Crocker, and K. T. Matteson. 1986. Performance, analysis and simulation of a two-well tracer test at the Mobile site. Water Resour. Res., in press.

Neuman, S. P. 1983. Statistical characterization of aquifer heterogeneities: an overview. In, Recent Trends in Hydrogeology, Geological Society of America, special paper 189, pp. 81-102.

Osiensky, J. L., G. V. Winter, and R. E. Williams. 1984. Monitoring and mathematical modeling of contaminated ground-water plumes in fluvial environments. Ground Water vol. 22, pp. 298-306.

Parr, A. D., F. J. Molz, and J. G. Melville. 1983. Field determination of aquifer thermal energy storage parameters. Ground Water v. 21, pp. 22-35.

Philip, J. R. 1980. Field heterogeneity: some basic issues. Water Resour. Res. v. 16, pp. 443-448.

Pickens, J. F., and G. E. Grisak. 1981. Scale-dependent dispersion in a stratified granular aquifer. Water Resour. Res. v. 17, pp. 1191-1211.

Pickens, J. F., J. A. Cherry, G. E. Grisak, W. F. Merritt, and B. A. Risto. 1978. Ground Water v. 16, pp. 322-237.

Schwartz, F. W. 1977. Macroscopic dispersion in porous media: the controlling factors. Water Resour. Res. v. 13, pp. 743-752.

Smith, L., and F. W. Schwartz. 1981. Mass transport 3. Role of hydraulic conductivity data in prediction. Water Resour. Res. v. 17, pp. 1463-1479.

Sposito, G., W. A. Jury, and V. K. Gupta. 1986. Fundamental problems in the stochastic convection-dispersion model of solute transport in aquifers and field soils. Water Resour. Res. v. 22, pp. 77-88.

Sudicky, E. A., J. A. Cherry, and E. O. Frind. 1985. Migration of contaminants in groundwater at a landfill: a case study 4. A natural gradient dispersion test. J. of Hydrology v. 63, pp. 81-108.

Winter, C. L. 1982. Asymptotic properties of mass transport in random porous media. Ph.D. dissertation. Univ. of Ariz., Tucson.